Supporting Information

Rh-Catalyzed Regioselective C-H Activation and C-C Bond Formation: Synthesis and Photophysical Studies of Indazolo[2,3-a]quinolines

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Experimental

General Information. $[Cp^*RhCl_2]_2$ and $Cu(OAc)_2 \cdot H_2O$ (>98%) were purchased from Aldrich and used as received. Indazoles[15] and alkynes[16] were prepared according to literature. Silica gel-G plates (Merck) were used for TLC analysis with a mixture of hexane and ethyl acetate as the eluent. Melting point of the products was measured on Büchi melting point apparatus, MP B-540. Open capillary tubes were used for the measurements and are uncorrected. The ^1H and ^{13}C spectra were recorded on Bruker 600 MHz and Varian Mercury Plus 400 MHz NMR instruments using TMS as an internal standard and $CDCl_3$ as a solvent. Mestrenova software was used throughout the spectral analysis. Chemical shifts are given in parts per million (δ-scale) and the coupling constants are given in Hertz. Q-Tof ESI-MS instrument (model HAB 273) was used for recording HRMS data. Infrared spectra were recorded on Perkin Elmer FT-IR instrument using KBr disc. UV-vis spectra were recorded on Agilent spectrophotometer and Fluorescence spectra were recorded on Cary Eclipse spectrofluorimeter.

General procedure for Rh(III)-catalyzed oxidative annulation of 2-aryl-2*H*-indazoles with alkynes. 2-Aryl-2*H*-indazole (0.25 mmol), alkyne (0.30 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.30 mmol), K_2CO_3 (0.25 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) were stirred at 100 °C for 6 h in $(CH_2Cl)_2$ under nitrogen atmosphere. The progress of the reaction was monitored by TLC using ethyl acetate and hexane as eluent. After completion, the reaction mixture was diluted with CH_2Cl_2 (30 mL) and washed with water (1 x 5 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was purified on silica gel column chromatography using a 1:50 ethyl acetate and hexane.

5,6-Diphenylindazolo[2,3-*a*]quinoline 3a.[6d] Yellow solid; 61 mg, yield 66%; mp 242-243 °C; R_f = 0.40 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 9.09 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.81 (t, *J* = 7.3 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.36–7.35 (m, 3H), 7.32-7.27 (m, 5H), 7.25-7.23 (m, 2H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 136.5, 136.5, 134.0, 133.6, 131.7, 131.2, 130.7, 130.3, 129.2, 128.5, 128.0, 128.0, 127.8, 127.6, 126.2, 125.7, 121.8, 120.5, 117.6, 117.4, 116.5; FT-IR (KBr) 3065, 3025, 2958, 2922, 2851, 1643, 1626, 1607, 1442, 1351, 1127, 1073, 805, 742 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{18}N_2+H]^+$ 371.1543, found 371.1546.

3-Chloro-5,6-diphenylindazolo[2,3-*a*]quinoline 3b. Yellow solid; 71 mg, yield 70%; mp 260-261 °C; R_f = 0.34 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.03 (d, *J* = 9.0 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.75 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.58 (d, *J* = 2.1 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.37-7.36 (m, 3H), 7.34-7.27 (m, 5H), 7.21 (d, *J* = 6.6 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.66 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 136.0, 135.6, 132.8, 132.0, 131.9, 131.8, 131.5, 131.0, 130.0, 129.4, 128.4, 128.1, 128.1, 127.9, 127.6, 126.9, 126.7, 121.6, 120.8, 118.9, 117.6, 116.4; FT-IR (KBr) 2960, 2919, 2850, 1638, 1540, 1485, 1383, 1224, 1147, 1085, 846, 752 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{17}ClN_2 + H]^+$ 405.1159, found 405.1156.

3-Ethyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3c. Yellow solid; 61 mg, yield 62%; mp 261-262 °C; R_f = 0.31 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00 (d, *J* = 8.6 Hz, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.68 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.40 (s, 1H), 7.37-7.34 (m, 3H), 7.33-7.28 (m, 5H), 7.25-7.23 (m, 2H), 6.90 (t, *J* = 7.2 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 1H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 142.5, 136.6, 136.6, 133.9, 131.9, 131.4, 131.2, 130.7, 130.4, 129.7, 128.5, 128.0, 127.9, 127.6, 127.4, 126.3, 125.7, 121.8, 120.3, 117.6, 117.4, 116.4, 29.06, 15.90; FT-IR (KBr) 3031, 2964, 2918, 2850, 1660, 1641, 1551, 1443, 1356, 1227, 1104, 1069 825, 744 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2 + H]^+$ 399.1861, found 399.1866.

3-*Iso*propyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3d. Yellow solid; 66 mg, yield 64%; mp 282-283 °C; R_f = 0.31 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.01 (d, *J* = 8.7 Hz, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.72 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 1.6 Hz, 1H), 7.38-7.34 (m, 3H), 7.33-7.30 (m, 2H), 7.29-7.27 (m, 3H), 7.25-7.23 (m, 2H), 6.90 (m, t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 8.5 Hz, 1H), 3.07-2.94 (sep, *J* = 6.9 Hz, 1H), 1.26 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 147.0, 136.7, 136.6, 134.0, 132.0, 131.4, 131.2, 130.6, 130.4, 128.5, 128.0, 127.97, 127.93, 127.6, 127.4, 125.6, 125.1, 121.8, 120.3, 117.6, 117.4, 116.4, 34.3, 24.2; FT-IR (KBr) 2960, 2919, 2851, 1637, 1557, 1462, 1384, 1358, 1261, 1105, 1068, 830, 743 cm^{-1}. HRMS (ESI) calcd for $[C_{30}H_{24}N_2 + H]^+$ 413.2018, found 413.2024.

3-Methyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3e. Yellow solid; 65 mg, yield 68%; mp 253-254 °C; R_f = 0.26 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (d,

J = 8.6 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.37-7.35 (m, 4H), 7.33-7.28 (m, 5H), 7.23-7.22 (m, 2H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 136.6, 136.6, 136.1, 133.8, 131.8, 131.4, 131.2, 130.9, 130.7, 130.3, 128.5, 128.0, 127.9, 127.6, 127.4, 127.4, 125.7, 121.7, 120.4, 117.6, 117.2, 116.4, 21.7; FT-IR (KBr) 2964, 2921, 2853, 1638, 1546, 1444, 1382, 1265, 1128, 1027, 808, 737 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2 + H]^+$ 385.1705, found 385.1700.

3-Methoxy-5,6-diphenylindazolo[2,3-*a*]quinoline 3f. Yellow solid; 76 mg, yield 76%; mp 240-241 °C; R_f = 0.54 (1:9 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.01 (d, *J* = 9.2 Hz, 1H), 7.93 (d, *J* = 8.6 Hz, 1H), 7.45-7.42 (m, 2H), 7.36-7.35 (m, 3H), 7.32-7.28 (m, 4H), 7.27-7.26 (m, 1H), 7.24-7.23 (m, 2H), 6.99 (d, *J* = 2.6 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.8, 149.5, 136.6, 136.5, 133.5, 131.2, 131.1, 130.9, 130.3, 128.5, 128.1, 128.0, 127.5, 127.4, 127.0, 121.6, 120.3, 118.9, 118.5, 117.7, 116.3, 109.2, 55.67; FT-IR (KBr) 2960, 2919, 2850, 1639, 1553, 1435, 1365, 1265, 1172, 1107, 1031, 845, 740 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2O + H]^+$ 401.1654, found 401.1658.

3-(Methylthio)-5,6-diphenylindazolo[2,3-a]quinoline 3g. Yellow solid; 76 mg, yield 73%; mp 251-252 °C; R_f = 0.27 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.99 (d, *J* = 8.8 Hz, 1H), 7.92 (d, *J* = 8.7 Hz, 1H), 7.69 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.44 (ddd, *J* = 8.6, 6.6, 1.0 Hz, 1H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.37-7.34 (m, 3H), 7.32-7.27 (m, 5H), 7.23-7.20 (m, 2H), 6.90 (ddd, *J* = 8.3, 6.7, 0.7 Hz, 1H), 6.66 (d, *J* = 8.5 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 136.9, 136.4, 136.1, 133.2, 131.4, 131.4, 131.3, 131.1, 130.3, 128.5, 128.1, 128.0, 127.8, 127.6, 126.2, 124.6, 121.7, 120.6, 117.9, 117.7, 116.4, 16.1; FT-IR (KBr) 3057, 2954, 2920, 2851, 1641, 1626, 1547, 1489, 1441, 1365, 1264, 1112, 1028, 848, 743 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2S + H]^+$ 417.1425, found 417.1431.

5,6-Diphenyl-3-(trifluoromethoxy)indazolo[2,3-a]quinoline 3h. Yellow solid; 98 mg, yield 86%; mp 107-108 °C; R_f = 0.39 (1:50 ethyl acetate/hexane);^{1}H NMR (600 MHz, $CDCl_3$) δ 9.13 (d, *J* = 9.2 Hz, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.67 (d, *J* = 9.3 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 1.9 Hz, 1H), 7.38-7.37 (m, 3H), 7.34-7.28 (m, 5H), 7.23-7.21 (m, 2H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz,

$CDCl_3$) δ 149.8, 147.0, 136.0, 135.6, 133.2, 132.1, 131.8, 131.7, 131.0, 130.1, 128.6, 128.3, 128.2, 128.1, 127.8, 126.8, 122.3, 122.3, 121.7, 121.5, 121.0, 119.7, 119.6, 119.3, 117.7, 116.6; ^{19}F NMR (376 Hz, DMSO-d_6) δ -57.1; FT-IR (KBr) 3082, 3062, 3043, 2925, 2852, 1628, 1553, 1445, 1435, 1258, 1219, 1170, 809, 753, 740 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{17}F_3N_2O$ +H]$^+$ 455.1371, found 455.1370.

5,6-Diphenyl-3-(trifluoromethyl)indazolo[2,3-a]quinoline 3i. Yellow solid; 73 mg, yield 67%; mp 225-226 °C; R_f = 0.39 (1:50 ethyl acetate/hexane);^{1}H NMR (600 MHz, $CDCl_3$) δ 9.20 (d, *J* = 8.8 Hz, 1H), 8.01 (dd, *J* = 8.8, 1.7 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.90 (s, 1H), 7.48 (ddd, *J* = 8.6, 6.6, 0.9 Hz, 1H), 7.38-7.37 (m, 3H), 7.35-7.28 (m, 5H), 7.23-7.21 (m, 2H), 6.94 (dd, *J* = 7.9, 6.8 Hz, 1H), 6.68 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.1, 135.97, 135.4, 135.1, 133.7, 132.3, 132.2, 131.1, 130.1, 128.6, 128.4, 128.3, 128.0 (q, $^2J_{C\text{-}F}$ = 31.8 Hz) 127.9, 125.3, 125.9 ($^1J_{C\text{-}F}$ = 274.0 Hz), 125.5 (q, $^3J_{C\text{-}F}$ = 4.2 Hz), 125.3 (q, $^3J_{C\text{-}F}$ = 2.9 Hz), 121.9, 121.2, 118.4, 117.7, 116.8; ^{19}F NMR (376 Hz, DMSO-d_6) δ -61.4; FT-IR (KBr) 3062, 2958, 2921, 2851, 1636, 1555, 1386, 1361, 1319, 1263, 1171, 1122, 1081, 822, 741 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{17}F_3N_2$ +H]$^+$ 439.1422, found 439.1418.

2-Chloro-5,6-diphenylindazolo[2,3-a]quinoline 3j. Yellow solid; 84 mg, yield 83%; mp 238-239 °C; R_f = 0.46 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.13 (d, *J* = 2.1 Hz, 1H), 7.96 (d, *J* = 8.7 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.50-7.47 (m, 2H), 7.39-7.38 (m, 3H), 7.35-7.30 (m, 5H), 7.24-7.23 (m, 2H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.9, 136.2, 136.0, 135.5, 133.9, 133.5, 132.1, 131.1, 130.9, 130.2, 129.4, 128.6, 128.2, 128.2, 127.7, 126.8, 124.1, 121.8, 120.9, 117.6, 117.2, 116.6; FT-IR (KBr) 3060, 2955, 2924, 2852, 1729, 1649, 1627, 1606, 1544, 1491, 1309, 1108, 1091, 817, 742 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{17}ClN_2$ +H]$^+$ 405.1159, found 405.1148.

2-Ethyl-5,6-diphenylindazolo[2,3-a]quinoline 3k. Yellow solid; 70 mg, yield 71%; mp 171-172 °C; R_f = 0.35 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.44 (ddd, *J* = 8.6, 6.6, 0.9 Hz, 1H), 7.34-7.35 (m, 4H), 7.31-7.25 (m, 5H), 7.23-7.21 (m, 2H), 6.90-6.88 (m, 1H), 6.67 (d, *J* = 8.5 Hz, 1H), 2.97 (q, *J* = 7.6 Hz, 2H), 1.41 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$)

δ 149.7, 146.5, 136.6, 136.6, 134.1, 133.6, 131.9, 131.2, 130.4, 129.8, 128.5, 128.0, 128.0, 127.9, 127.8, 127.4, 126.8, 123.7, 121.9, 120.3, 117.5, 116.4, 115.9, 29.4, 15.9; FT-IR (KBr) 3059, 3025, 2966, 2931, 2871, 1619, 1541, 1500, 1441, 1363, 1309, 1233, 1181, 1072, 1029, 828, 737 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2 +H]^+$ 399.1861, found 399.1870.

2-Methyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3l. Yellow solid; 56 mg, yield 59%; mp 252-253 °C; R_f = 0.27 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 8.90 (s, 1H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.36-7.33 (m, 4H), 7.31-7.27 (m, 5H), 7.22-7.23 (m, 2H), 6.90 (t, *J* = 7.2 Hz, 1H), 6.67 (d, *J* = 8.4 Hz, 1H), 2.68 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 140.2, 136.6, 136.6, 134.1, 133.5, 131.9, 131.2, 130.4, 129.7, 128.5, 128.0, 127.9, 127.9, 127.8, 127.4, 123.5, 121.9, 120.3, 117.5, 117.0, 116.4, 22.0; FT-IR (KBr) 2960, 2920, 2849, 1641, 1553, 1442, 1384, 1261, 1173, 1104, 1024, 805, 737 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2 +H]^+$ 385.1705, found 385.1696.

2-Methoxy-5,6-diphenylindazolo[2,3-*a*]quinoline 3m and 4-methoxy-5,6-diphenylindazolo[2,3-*a*]quinoline 3m' (Regioisomers).Yellow solid; 68 mg, yield 68%; mp 222-223 °C; R_f = 0.46 (1:9 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.5 Hz, 1H), 8.48 (d, *J* = 2.5 Hz, 1H), 7.94 (d, *J* = 8.8 Hz, 1H), 7.91 (s, 1H), 7.75 (t, *J* = 8.2 Hz, 1H), 7.52 (d, *J* = 9.0 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.43-7.42 (m, 1H), 7.36-7.35 (m, 5H), 7.31-7.25 (m, 10H), 7.23-7.20 (m, 3H), 7.17-7.10 (m, 3H), 6.95 (d, *J* = 7.9 Hz, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.1 Hz, 1H), 6.69 (d, *J* = 8.4 Hz, 1H), 6.49 (d, *J* = 8.5 Hz, 1H), 4.12 (s, 3H), 3.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.9, 158.0, 149.8, 149.8, 140.7, 136.6, 136.6, 134.8, 134.2, 132.3, 131.8, 131.2, 130.6, 130.5, 130.0, 129.7, 129.5, 128.5, 128.3, 128.2, 128.0, 127.9, 127.9, 127.6, 127.4, 126.6, 125.8, 122.6, 122.0, 121.9, 120.5, 120.4, 120.2, 119.7, 118.1, 117.5, 117.4, 117.2, 116.4, 116.2, 114.1, 113.1, 110.3, 108.1, 106.9, 98.3, 56.2, 56.0; FT-IR (KBr) 2962, 2925, 2849, 1737, 1629, 1612, 1516, 1493, 1362, 1258, 1148, 1026, 843, 739 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2O +H]^+$ 401.1654, found 401.1636.

2,3-Dimethyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3n. Yellow solid; 71 mg, yield 71%; mp 274-275 °C; R_f = 0.20 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 8.86 (s, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.43 (ddd, *J* = 8.6, 6.6, 1.1 Hz, 1H), 7.35- 7.34 (m, 4H),

7.32-7.26 (m, 5H), 7.23-7.21 (m, 2H), 6.88 (ddd, J = 8.4, 6.6, 0.8 Hz, 1H), 6.66 (d, J = 8.5 Hz, 1H), 2.58 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 139.6, 136.7, 136.7, 135.7, 133.8, 132.0, 131.6, 131.2, 130.5, 129.7, 128.4, 128.0, 127.9, 127.8, 127.6, 127.3, 123.8, 121.8, 120.2, 117.5, 117.5, 116.3, 20.5, 20.2; FT-IR (KBr) 2953, 2920, 2849, 1638, 1542, 1491, 1441, 1263, 1148, 1108, 1072, 816, 741 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2 + H]^+$ 399.1861, found 399.1848.

5,6-Diphenyl-[1,3]dioxolo[4,5-*g*]indazolo[2,3-*a*]quinoline 3o. Yellow solid; 85 mg, yield 82%; mp 294-295 °C; R_f = 0.15 (1:50 ethyl acetate/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, J = 8.9 Hz, 1H), 7.90 (d, J = 8.7 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.37-7.33 (m, 4H), 7.26-7.23 (m, 2H), 7.19 (m, 5H), 6.88 (t, J = 7.6 Hz, 1H), 6.53 (d, J = 8.5 Hz, 1H), 5.83 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.5, 145.6, 143.9, 137.4, 136.1, 131.4, 130.8, 130.6, 130.4, 130.1, 129.3, 128.4, 127.9, 127.6, 127.13, 127.07, 121.6, 120.7, 117.9, 116.4, 112.2, 111.0, 110.8, 101.8; FT-IR (KBr) 3061, 3025, 2958, 2922, 2852, 1740, 1637, 1548, 1491, 1450, 1367, 1269, 1127, 1105, 1039, 806, 742 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{18}N_2O_2 + H]^+$ 415.1447, found 415.1432.

1-Methyl-5,6-diphenylindazolo[2,3-*a*]quinoline 3p. Yellow solid; 77 mg, yield 80%; mp 207-208 °C; R_f = 0.55 (1:50 ethyl acetate/hexane);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.7 Hz, 1H), 7.57 (d, J = 7.2 Hz, 1H), 7.44-7.39 (m, 2H), 7.36-7.30 (m, 4H), 7.30-7.25 (m, 5H), 7.21-7.19 (m, 2H), 6.89-6.85 (m, 1H), 6.58 (d, J = 8.5 Hz, 1H), 3.47 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.9, 137.3, 136.8, 134.3, 133.4, 132.7, 132.7, 131.2, 130.6, 130.6, 130.3, 128.5, 128.0, 127.8, 127.4, 127.3, 127.1, 126.1, 125.3, 121.6, 120.4, 116.8, 116.3, 26.1; FT-IR (KBr) 2966, 2924, 2852, 1645, 1628, 1550, 1493, 1441, 1363, 1304, 1263, 1154, 1104, 1026 797, 741 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2+H]^+$ 385.1705, found 385.1695.

6,7-Diphenyl-2,3-dihydro-1*H*-cyclopenta[*h*]indazolo[2,3-*a*]quinoline 3q. Yellow solid; 76 mg, yield 74%; mp 234-235 °C; R_f = 0.50 (1:50 ethyl acetate/hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 8.7 Hz, 1H), 7.40 (ddd, J = 8.7, 6.6, 1.1 Hz, 1H), 7.37 (d, J = 1.7 Hz, 2H), 7.35-7.30 (m, 3H), 7.29-7.24 (m, 5H), 7.22-7.19 (m, 2H), 6.86 (ddd, J = 8.5, 6.6, 0.8 Hz, 1H), 6.61 (d, J = 8.5 Hz, 1H), 4.23 (t, J = 7.4 Hz, 2H), 3.16 (t, J = 7.7 Hz, 2H), 2.33 (p, J = 7.6 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.4, 147.3, 137.4, 136.9, 134.5,

134.3, 132.4, 131.6, 131.1, 130.4, 129.6, 128.4, 128.0, 127.8, 127.2, 127.1, 126.5, 125.4, 122.7, 121.7, 120.2, 116.7, 116.6, 36.6, 33.6, 25.6; FT-IR (KBr) 3058, 2962, 2921, 2843, 1629, 1549, 1495, 1440, 1380, 1260, 1106, 1070, 820, 735 cm^{-1}. HRMS (ESI) calcd for $[C_{30}H_{22}N_2+H]^+$ 411.1861, found 411.1845.

7,8-Diphenylbenzo[*h*]indazolo[2,3-*a*]quinoline 3r. Yellow solid; 61 mg, yield 58%; mp 170-171 °C; R_f = 0.42 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 11.46 (d, *J* = 8.8 Hz, 1H), 8.11 (d, *J* = 8.6 Hz, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 8.00 (t, *J* = 7.3 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.82 (t, *J* = 7.4 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.40-7.37 (m, 3H), 7.35-7.30 (m, 5H), 7.28-7.26 (m, 2H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.5, 137.4, 136.7, 134.4, 134.0, 131.3, 131.2, 130.3, 129.7, 129.14, 129.11, 128.5, 128.3, 128.1, 128.0, 127.8, 127.8, 127.7, 127.66, 127.62, 127.4, 125.4, 124.9, 124.4, 121.8, 120.4, 116.6, 116.0; FT-IR (KBr) 2962, 2921, 2851, 1635, 1548, 1475, 1362, 1442, 1263, 1195, 1165, 1027, 824, 748 cm^{-1}. HRMS (ESI) calcd for $[C_{31}H_{20}N_2+H]^+$ 421.1705, found 421.1706.

5,6-Diphenylindazolo[2,3-*a*][1,6]naphthyridine 3s. Yellow solid; 73 mg, yield 79%; mp 209-210 °C; R_f = 0.27 (1:4 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 8.90 (d, *J* = 5.7 Hz, 1H), 8.83 (d, *J* = 5.7 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.49 (ddd, *J* = 8.7, 6.6, 1.0 Hz, 1H), 7.39-7.38 (m, 3H), 7.34-7.29 (m, 5H), 7.26-7.25 (m, 2H), 6.95 (ddd, *J* = 8.4, 6.6, 0.6 Hz, 1H), 6.69 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.4, 150.6, 147.9, 137.6, 135.7, 134.7, 133.1, 132.5, 132.2, 131.2, 130.2, 128.8, 128.7, 128.4, 128.3, 128.0, 121.9, 121.5, 120.9, 117.6, 117.0, 110.5; FT-IR (KBr) 2964, 2924, 2853, 1631, 1598, 1479, 1436, 1347, 1310, 1262, 1183, 1031, 826, 745 cm^{-1}. HRMS (ESI) calcd for $[C_{26}H_{17}N_3+H]^+$ 372.1501, found 372.1505.

8-Fluoro-5,6-diphenylindazolo[2,3-*a*]quinoline 3t. Yellow solid; 72 mg, yield 74%; mp 231-232 °C; R_f = 0.27 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 9.03 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.90 (dd, *J* = 9.3, 4.6 Hz, 1H), 7.79 (ddd, *J* = 8.4, 7.1, 1.3 Hz, 1H), 7.61 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.52-7.49 (m, 1H), 7.37-7.35 (m, 3H), 7.31-7.21 (m, 8H), 6.24 (dd, *J* = 9.7, 2.3 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.3 (d, $^1J_{C\text{-}F}$ = 238.2 Hz), 146.9, 136.3, 136.1, 133.7 (d, $^3J_{C\text{-}F}$ = 13.7 Hz), 131.2, 130.6, 130.2, 129.8, 129.3, 128.6, 128.2, 128.08, 128.06, 127.5, 126.4, 125.7, 121.04, 118.8, (d, $^2J_{C\text{-}F}$ = 28.3 Hz), 118.3 (d,

$^{3}J_{C\text{-}F}$ = 9.5 Hz), 117.2, 105.0 (d, $^{2}J_{C\text{-}F}$ = 25.6 Hz); ^{19}F NMR (376 Hz, DMSO-d_6) δ -120.3; FT-IR (KBr) 3054, 3026, 2921, 2852, 1633, 1588, 1545, 1524, 1491, 1434, 1275, 1198, 1098, 761 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{17}FN_2+H]^+$ 389.1454, found 389.1438.

8-Methoxy-5,6-diphenylindazolo[2,3-*a*]quinoline 3u. Yellow solid; 68 mg, yield 68%; mp 229-230 °C; R_f = 0.29 (1:9 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00-8.99 (m, 1H), 7.84 (d, *J* = 9.2 Hz, 1H), 7.77 (ddd, *J* = 8.4, 7.1, 1.3 Hz, 1H), 7.59 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.48 (ddd, *J* = 8.2, 7.1, 1.1 Hz, 1H), 7.39-7.25 (m, 10H), 7.14 (dd, *J* = 9.3, 2.4 Hz, 1H), 5.81 (d, *J* = 2.4 Hz, 1H), 3.44 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.0, 146.2, 136.6, 136.6, 133.8, 132.7, 131.3, 131.0, 130.7, 130.5, 129.0, 128.4, 128.0, 127.9, 127.8, 127.4, 125.9, 125.6, 121.9, 117.9, 117.4, 117.0, 99.0, 55.0; FT-IR (KBr) 2952, 2923, 2853, 1638, 1548, 1522, 1489, 1435, 1384, 1213, 1169, 1105, 1072, 812, 754 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{20}N_2O+H]^+$ 401.1654, found 401.1658.

8,9-Dimethoxy-5,6-diphenylindazolo[2,3-*a*]quinoline 3v. Yellow solid; 77 mg, yield 72%; mp 256-257 °C; R_f = 0.29 (1:4 ethyl acetate/hexane);^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (d, *J* = 8.6 Hz, 1H), 7.78-7.73 (m, 1H), 7.57 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.46-7.41 (m, 1H), 7.40-7.34 (m, 2H), 7.28-7.33 (m, 5H), 7.27-7.24 (m, 4H), 5.80 (s, 1H), 4.00 (s, 3H), 3.49 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.3, 146.45, 146.40, 136.7, 136.6, 133.9, 133.1, 131.25, 131.20, 130.6, 130.2, 129.1, 128.4, 128.02, 128.0, 127.8, 127.4, 125.4, 125.0, 116.6, 111.3, 99.5, 95.3, 56.1, 55.5; FT-IR (KBr) 3002, 2960, 2921, 2853, 2833, 1639, 1545, 1496, 1463, 1441, 1159, 1099, 836, 737 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2O_2+H]^+$ 431.1760, found 431.1768.

5,6-Bis(4-bromophenyl)indazolo[2,3-*a*]quinoline 3ab. Yellow solid; 99 mg, yield 75%; mp 243-244 °C; R_f = 0.30 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.3 Hz, 1H), 7.96 (d, *J* = 8.7 Hz, 1H), 7.82 (ddd, *J* = 8.4, 6.7, 1.7 Hz, 1H), 7.56-7.50 (m, 4H), 7.49-7.46 (m, 3H), 7.18-7.15 (m, 2H), 7.10-7.08 (m, 2H), 6.97 (ddd, *J* = 8.4, 6.6, 0.7 Hz, 1H), 6.73 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 135.2, 135.1, 133.6, 132.7, 132.7, 132.0, 131.9, 131.6, 131.0, 129.7, 129.5, 128.0, 127.7, 126.4, 125.1, 122.6, 122.1, 121.4, 121.0, 117.5, 117.4, 116.8; FT-IR (KBr) 2960, 2919, 2847, 1641, 1544, 1488, 1387, 1130, 1072, 827, 742 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{16}Br_2N_2+H]^+$ 526.9758, found 526.9761.

5,6-Bis(4-chlorophenyl)indazolo[2,3-*a*]quinoline 3ac. Yellow solid; 79 mg, yield 72%; mp 244-245 °C; R_f = 0.30 (1:50 ethyl acetate/hexane);^{1}H NMR (600 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.82 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.55 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.52 (ddd, *J* = 8.2, 6.9, 1.1 Hz, 1H), 7.47 (ddd, *J* = 8.6, 6.6, 1.0 Hz, 1H), 7.38-7.36 (m, 2H), 7.33-7.30 (m, 2H), 7.23-7.21 (m, 2H), 7.16-7.13 (m, 2H), 6.96 (ddd, *J* = 8.4, 6.6, 0.8 Hz, 1H), 6.73 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 134.7, 134.3, 133.8, 133.6, 132.8, 132.4, 131.7, 131.1, 129.6, 129.6, 129.1, 128.6, 128.0, 127.7, 126.4, 125.2, 121.4, 121.0, 117.5, 117.4, 116.8; FT-IR (KBr) 3063, 2961, 2924, 2853, 1904, 1731, 1628, 1599, 1521, 1494, 1390, 1145, 1091, 830, 752 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{16}Cl_2N_2+H]^+$ 439.0769, found 439.0773.

5,6-Bis(4-fluorophenyl)indazolo[2,3-*a*]quinoline 3ad. Yellow solid; 80 mg, yield 79%; mp 245-246 °C; R_f = 0.27 (1:50 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.81 (ddd, *J* = 8.3, 7.1, 1.3 Hz, 1H), 7.58-7.56 (m, 1H), 7.53-7.51 (m, 1H), 7.47-7.45 (m, 1H), 7.26-7.23 (m, 2H), 7.18-7.16 (m, 2H), 7.08 (t, *J* = 8.6 Hz, 2H), 7.02 (t, *J* = 8.6 Hz, 2H), 6.95 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.5 (d, $^1J_{C\text{-}F}$ = 248.1 Hz), 162.2 (d, $^1J_{C\text{-}F}$ = 247.5 Hz), 149.7, 133.6, 133.2, 132.8 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 132.3 (d, $^4J_{C\text{-}F}$ = 3.5 Hz), 132.2 (d, $^4J_{C\text{-}F}$ = 3.5 Hz), 132.0 (d, $^3J_{C\text{-}F}$ = 8.1 Hz), 131.4, 130.0, 129.5, 127.9, 127.8, 126.4, 125.5, 121.5, 120.8, 117.5, 117.5, 116.7, 115.8 (d, $^2J_{C\text{-}F}$ = 21.5 Hz), 115.3 (d, $^2J_{C\text{-}F}$ = 21.5 Hz); ^{19}F NMR (376 Hz, DMSO-d_6) δ -114.2, -113.2; FT-IR (KBr) 2960, 2921, 2852, 1629, 1602, 1549, 1504, 1429, 1354, 1223, 1154, 1093, 829, 744 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{16}F_2N_2+H]^+$ 407.1360, found 407.1365.

5,6-Bis(4-methoxyphenyl)indazolo[2,3-*a*]quinoline 3ae. Yellow solid; 78 mg, yield 73%; mp 246-247 °C; R_f = 0.36 (1:9 ethyl acetate/hexane); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.79 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.65 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.51 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.45 (ddd, *J* = 8.6, 6.6, 1.0 Hz, 1H), 7.21-7.19 (m, 2H), 7.14-7.12 (m, 2H), 6.94-6.89 (m, 3H), 6.87-6.84 (m, 2H), 6.78 (d, *J* = 8.5 Hz, 1H), 3.86 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.1, 158.7, 149.7, 134.1, 133.5, 132.3, 132.2, 131.5, 130.7, 129.1, 129.0, 128.8, 128.0, 127.8, 126.1, 126.0, 122.0, 120.4, 117.6, 117.3, 116.5, 113.9, 113.5, 55.36, 55.34; FT-IR (KBr)

2997, 2958, 2922, 2851, 1737, 1651, 1628, 1607, 1510, 1459, 1243, 1175, 1107, 1027, 830, 746 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2O_2+H]^+$ 431.1760, found 431.1763.

5,6-Di-*p*-tolylindazolo[2,3-*a*]quinoline 3af. Yellow solid; 71 mg, yield 71%; mp 259-260 °C; R_f = 0.35 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 9.07 (dd, *J* = 8.5, 0.8 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.78 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.61 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.49 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.44 (ddd, *J* = 8.6, 6.6, 1.1 Hz, 1H), 7.18-7.15 (m, 4H), 7.13-7.10 (m, 4H), 6.91 (ddd, *J* = 8.4, 6.6, 0.8 Hz, 1H), 6.71-6.69 (m, 1H), 2.40 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 137.5, 136.9, 134.1, 133.6, 133.52, 133.51, 132.1, 131.0, 130.8, 130.1, 129.2, 129.1, 128.7, 128.1, 127.7, 126.1, 125.9, 122.0, 120.4, 117.6, 117.3, 116.5, 21.58, 21.44; FT-IR (KBr) 3056, 3027, 2962, 2920, 1640, 1622, 1546, 1503, 1304, 1187, 1108, 1019, 818, 740 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2+H]^+$ 399.1861, found 399.1866.

5,6-Bis(3-chlorophenyl)indazolo[2,3-*a*]quinoline 3ag. Yellow solid; 73 mg, yield 67%; mp 281-282 °C; R_f = 0.32 (1:50 ethyl acetate/hexane); 1:1 mixture of rotomers; ^1H NMR (600 MHz, $CDCl_3$) δ 9.09 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.7 Hz, 1H), 7.84 (t, *J* = 7.5 Hz, 1H), 7.58-7.54 (m, 2H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.36-7.33 (m, 1H), 7.32-7.29 (m, 2H), 7.27-7.24 (m, 2H), 7.20 (d, *J* = 7.2 Hz, 1H), 7.14-7.10 (m, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.72 (dd, *J* = 8.3, 2.9 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 138.0, 137.9, 134.7, 134.5, 134.3, 134.1, 133.6, 132.5, 131.1, 131.0, 130.9, 130.30, 130.27, 130.1, 129.9, 129.8, 129.6, 129.5, 129.41, 129.40, 129.38, 129.34, 128.59, 128.55, 128.52, 128.08, 128.06, 128.0, 127.7, 126.5, 125.0, 121.4, 121.1, 117.5, 117.4, 116.8; FT-IR (KBr) 2962, 2921, 2851, 2096, 1639, 1497, 1472, 1433, 1351, 1308, 1183, 1096, 789, 736 cm^{-1}. HRMS (ESI) calcd for $[C_{27}H_{16}Cl_2N_2+H]^+$ 439.0769, found 439.0774.

5,6-Di-*m*-tolylindazolo[2,3-*a*]quinoline 3ah. Yellow solid; 82 mg, yield 83%; mp 212-213 °C; R_f = 0.37 (1:50 ethyl acetate/hexane); 1:1 mixture of rotomers; ^1H NMR (600 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 8.7 Hz, 2H), 7.81-7.80 (m, 2H), 7.63-7.62 (m, 2H), 7.52-7.50 (m, 2H), 7.44 (dd, *J* = 11.5, 3.9 Hz, 2H), 7.25-7.24 (m, 2H), 7.21-7.17 (m, 2H), 7.16 (d, *J* = 7.7 Hz, 2H), 7.11-7.02 (m, 10H), 6.93-6.88 (m, 2H), 6.69 (d, *J* = 8.5 Hz, 2H), 2.31-2.30 (m, 9H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 137.99, 137.95, 137.5, 137.4, 136.39, 136.38, 134.09, 134.07, 133.5, 131.88, 131.86, 130.9, 130.8, 129.1, 128.65, 128.64, 128.30, 128.28, 128.27, 128.1, 127.8, 127.7, 127.7, 127.3, 126.1,

125.8, 122.0, 121.2, 120.4, 117.6, 117.3, 116.5, 21.57, 21.56, 21.54, 21.53; FT-IR (KBr) 2953, 2921, 2853, 1793, 1731, 1629, 1522, 1488, 1308, 1261, 1103, 1033, 790, 733 cm^{-1}. HRMS (ESI) calcd for $[C_{29}H_{22}N_2+H]^+$ 399.1861, found 399.1865.

5,6-Di(naphthalen-1-yl)indazolo[2,3-*a*]quinoline 3ai. Yellow solid; 87 mg, yield 74%; mp 301-302 °C; R_f = 0.17 (1:50 ethyl acetate/hexane); 10:1 mixture of rotomers; ^1H NMR (600 MHz, $CDCl_3$) δ 9.18 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.85-7.81 (m, 3H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.47-7.35 (m, 5H), 7.32-7.29 (m, 1H), 7.26 (d, *J* = 6.9 Hz, 1H), 7.18 (d, *J* = 6.3 Hz, 1H), 7.15-7.08 (m, 3H), 6.67-6.64 (m, 1H), 5.99 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8, 134.1, 134.0, 133.6, 133.4, 133.3, 133.2, 132.3, 132.2, 130.0, 129.5, 128.6, 128.5, 128.4, 128.34, 128.32, 127.8, 127.6, 126.7, 126.6, 126.42, 126.41, 126.4, 126.1, 126.0, 125.9, 125.7, 125.5, 125.2, 121.4, 120.9, 117.4, 117.4, 116.5; FT-IR (KBr) 2962, 2920, 2853, 1638, 1468, 1384, 1261, 1222, 1091, 1015, 802, 742 cm^{-1}. HRMS (ESI) calcd for $[C_{35}H_{22}N_2+H]^+$ 471.1861, found 471.1861.

5-(4-methoxyphenyl)-6-phenylindazolo[2,3-a]quinolone 3aj and 6-(4-methoxyphenyl)-5-phenylindazolo[2,3-a]quinoline 3aj'. (Regioisomers). Yellow solid; 78 mg, yield 78%; mp 222-223 °C; R_f = 0.54 (1:50 ethyl acetate/hexane); ^1H NMR (600 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.4, 2H), 7.96-7.93 (m, 2H), 7.81-7.80 (m, 2H), 7.66 (dd, *J* = 8.3, 1.3, 1H), 7.60 (dd, *J* = 8.3, 1.3, 1H), 7.52-7.50 (m, 2H), 7.46-7.44 (m, 2H), 7.38-7.37 (m, 3H), 7.34- 7.29 (m, 5H), 7.24-7.22 (m, 2H), 7.22-7.22 (m, 2H), 7.15-7.13 (m, 2H), 6.95-6.88 (m, 4H), 6.85-6.83 (m, 2H), 6.80-6.78 (m, 1H), 6.66 (d, *J* = 8.5, 1H), 3.85 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.1, 158.8, 149.7, 136.7, 136.6, 134.3, 133.8, 133.5, 133.5, 132.3, 132.1, 131.8, 131.5, 131.2, 130.9, 130.4, 130.3, 129.2, 129.1, 128.7, 128.6, 128.5, 128.1, 128.0, 127.9, 127.8, 127.4, 126.1, 126.0, 125.7, 121.9, 121.8, 120.5, 120.4, 117.7, 117.5, 117.3, 116.5, 116.5, 113.9, 113.5, 55.34, 55.32; FT-IR (KBr) 2924, 2853, 1649, 1624, 1606, 1458, 1244, 1028, 740 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{21}N_2O+H]^+$ 401.1654, found 401.1686.

5,6-Dipropylindazolo[2,3-*a*]quinoline 3al. Yellow solid; 47 mg, yield 63%; mp 125-126 °C; R_f = 0.30 (1:50 ethyl acetate/hexane); ^1H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, *J* = 8.0 Hz, 1H), 8.07 (t, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.74-7.72 (m, 1H), 7.63-7.62 (m, 1H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.26-7.23 (m, 1H), 3.30-3.29 (m, 2H), 3.13-3.11 (m, 2H),

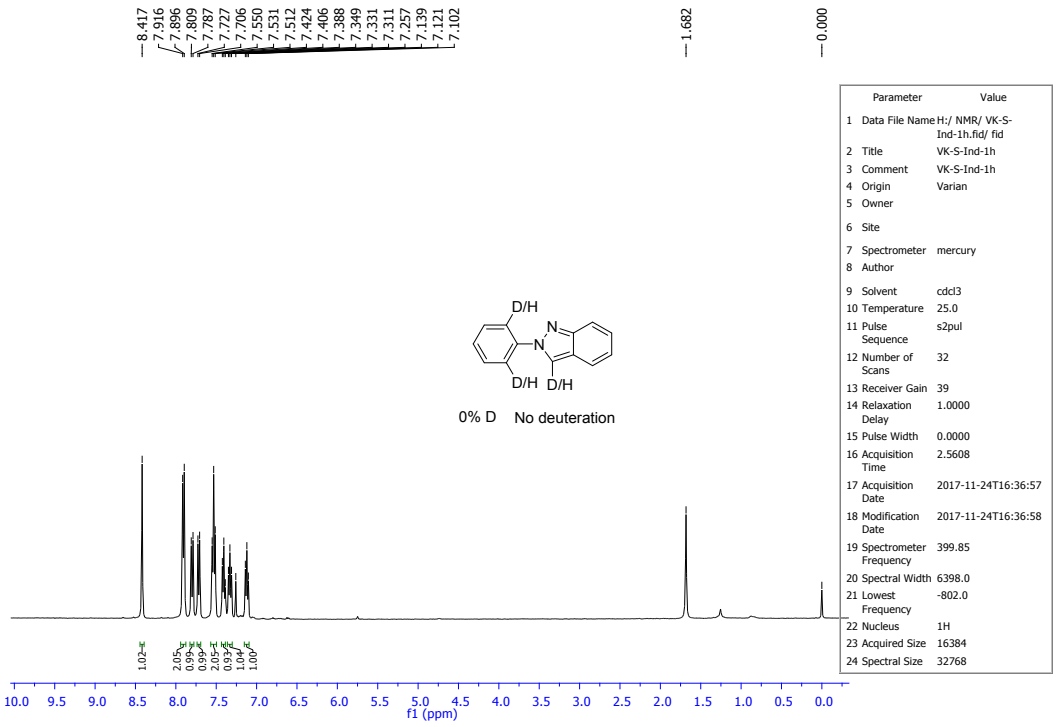
1.87-1.85 (m, 2H), 1.77-1.75 (m, 2H), 1.24-1.23 (m, 3H), 1.16 (t, J = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 133.3, 132.2, 131.4, 129.8, 128.2, 127.4, 126.1, 125.0, 124.9, 121.8, 120.7, 117.9, 116.9, 116.4, 31.5, 29.9, 24.4, 22.9, 14.8, 14.6; FT-IR (KBr) 3079, 2956, 2924, 2868, 1626, 1553, 1517, 1458, 1364, 1263, 1148, 1089, 884, 737 cm^{-1}. HRMS (ESI) calcd for $[C_{21}H_{22}N_2+H]^+$ 303.1861, found 303.1863.

Synthesis of 2-(4-Methylphenyl-2,6-*d*$_2$)-2*H*-indazole 1e-*d*$_2$. 2-Bromobenzaldehyde (0.5 mmol) and *p*-toluidine-d_2 aniline 84% D (0.6 mmol) were stirred in DMSO (5 mL) at room temperature for 0.25 h. The resultant mixture was treated with NaN_3 (0.75 mmol), CuI (15 mol%) and TMEDA (15 mol%) and stirred at 120 °C for 12 h. The progress of the reaction was monitored by TLC using ethyl acetate and hexane. After completion, the reaction mixture was cooled to room temperature and poured in ice cold water. The mixture was extracted using EtOAc (3 x 40 mL) and dried over Na_2SO_4. The solution was passed through a short pad of cellite and evaporated on a rotary evaporator to produce a residue that was purified on silica gel column chromatography using 1:50 ethyl acetate and hexane to give **1e-*d*$_2$** as a colorless solid with 82% D and 74% yield (163 mg). R_f = 0.26 (1:50 ethyl acetate/hexane); mp 99-100 °C;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.80-7.37 (m, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.34-7.30 (m, 3H), 7.12-7.10 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8, 138.0, 130.2, 130.1, 126.8, 122.8, 122.4, 120.9, 120.5, 120.4, 118.0, 21.2; FT-IR (KBr) 3118, 3043, 2920, 2853, 1624, 1517, 1488, 1448, 1378, 1194, 1034, 792, 739 cm^{-1}. HRMS (ESI) calcd for $[C_{14}H_{10}D_2N_2+H]^+$ 211.1204, found 211.1208.

Mechanistic investigation

Competition experiment using 1f and 1i. 2-(4-Methoxyphenyl)-2*H*-indazole **1f** (0.125 mmol), 2-(4-(trifluoromethyl)phenyl)-2*H*-indazole **1i** (0.125 mmol), 1,2-diphenylethyne **2a** (0.14 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.30 mmol), K_2CO_3 (0.25 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) were stirred at 100 °C for 6 h in $(CH_2Cl)_2$ under nitrogen atmosphere. The progress of the reaction was monitored by TLC using ethyl acetate and hexane as an eluent. The reaction mixture was cooled to room temperature and diluted with CH_2Cl_2 (30 mL) and washed with water (1 x 5 mL). Drying (Na_2SO_4) and evaporation of the solvent in vacuo provided a residue that was purified by column chromatography on silica gel using a 1:50 ethyl aceate and hexane as an eluent.

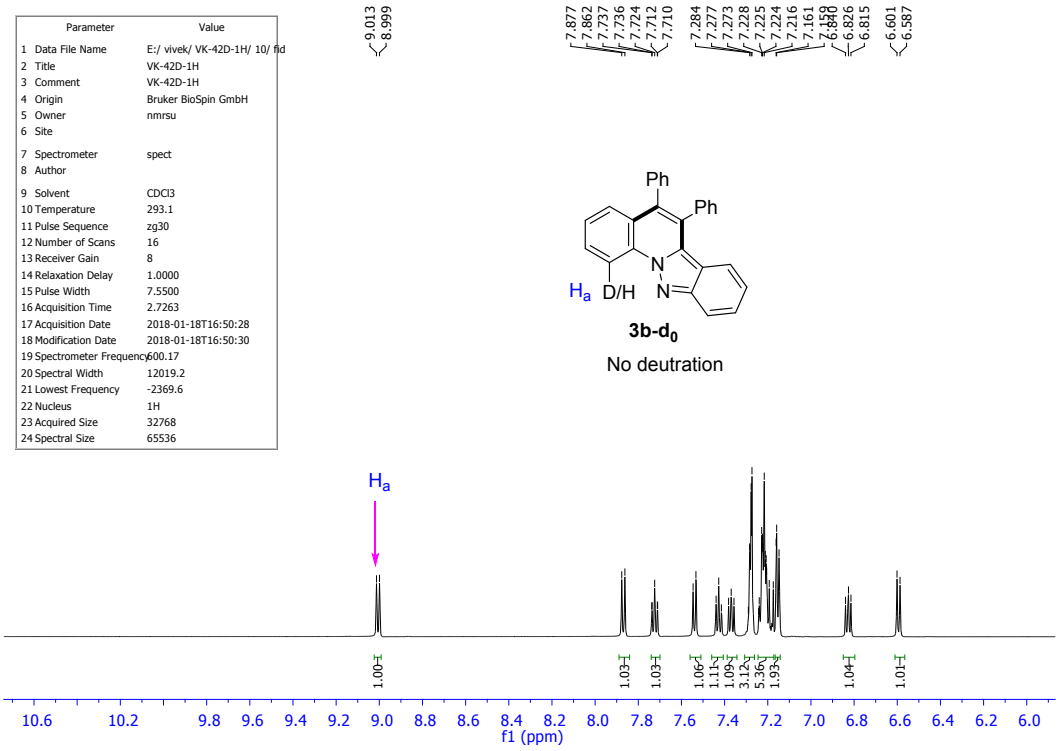
Rh(III)-catalyzed H/D exchange studies in DCE:D_2O. To a stirred solution of 2-aryl-2*H*-indazole (0.25 mmol), 1,2-diphenylethyne (0.30 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.30 mmol), K_2CO_3 (0.25 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) in $(CH_2Cl)_2$ (2 mL) under nitrogen atmosphere was added D_2O (1 mmol). The resultatnt mixture was stirred at 100 °C for 6 h and then cooled to room temperature. The reaction mixture was diluted with CH_2Cl_2 (25 mL) and the organic layer was washed with water (5 mL). Drying (Na_2SO_4) and evaporation of the solvents gave a residue that was purified on silica gel column chromatography using a 1:50 ethyl acetate and hexane as the eluent. ^1H NMR (600 MHz) analysis showed no deutration incorporation.



Rh(III)-Catalyzed H/D Exchange in DCE:D_2O

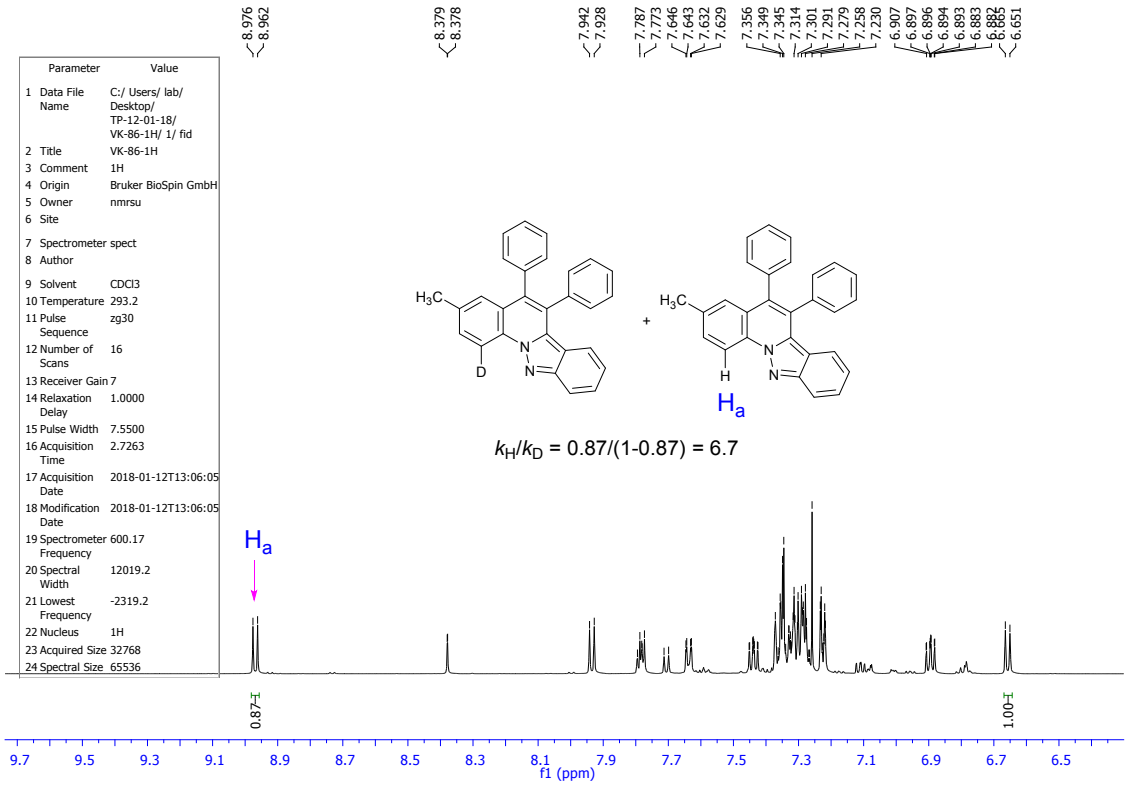
Rh(III)-catalyzed H/D exchange studies in DCE:D_2O in the presence of alkyne. To stirred solution of 2-aryl-2*H*-indazole (0.25 mmol), 1,2-diphenylethyne (0.30 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.30 mmol), K_2CO_3 (0.25 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) in $(CH_2Cl)_2$ (2 mL) under nitrogen atmosphere was added D_2O (1 mmol). The resultatnt mixture was

stirred at 100 °C for 6 h and then cooled to room temperature. The reaction mixture was diluted with CH_2Cl_2 (25 mL) and the organic layer was washed with water (5 mL). Drying (Na_2SO_4) and evaporation of the solvents gave a residue that was purified on silica gel column chromatography using a 1:50 ethyl acetate and hexane as the eluent. ^{1}H NMR (600 MHz) analysis showed no deutration incorporation.



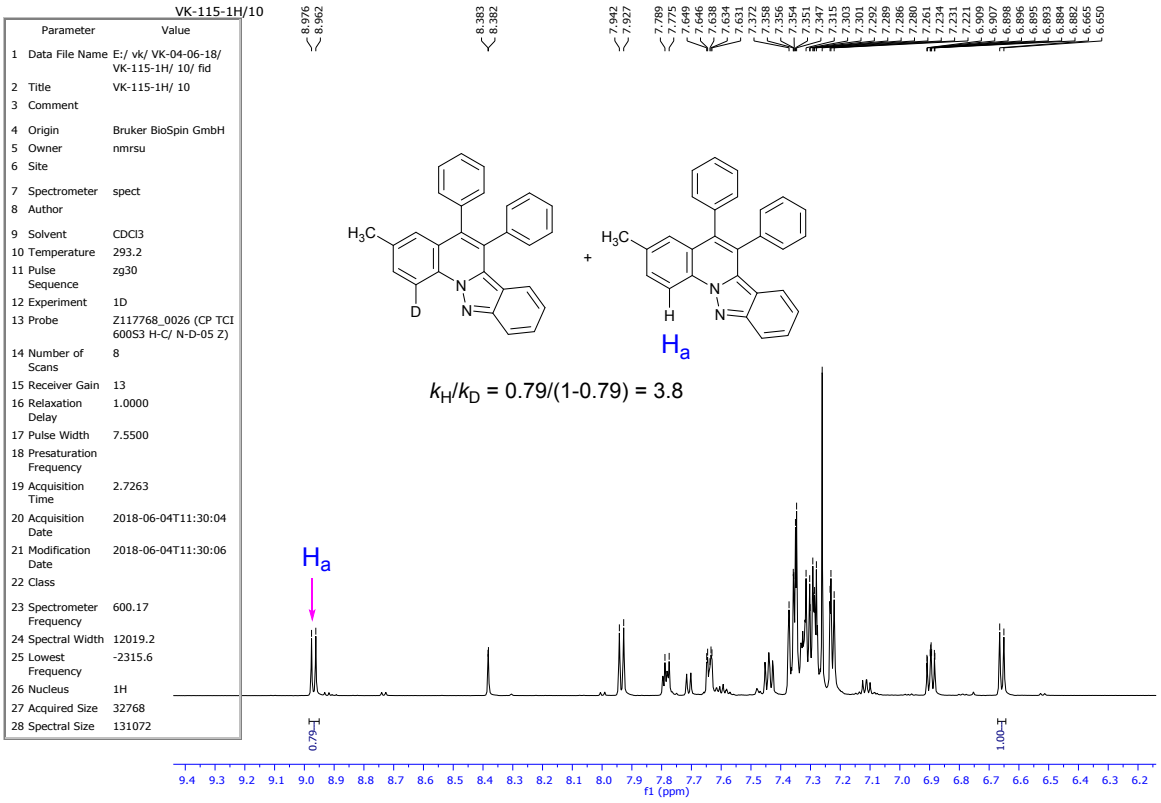
Rh(III)-Catalyzed H/D Exchange in DCE:D_2O in the presence of Alkyne

Kinetic isotope experiment in one pot competition reaction. 2-(4-Methylphenyl-2,6-d_2)-2*H*-indazole (0.125 mmol), 2-(*p*-tolyl)-2*H*-indazole (0.125 mmol), 1,2-diphenylethyne (0.20 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.30 mmol), K_2CO_3 (0.25 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) were stirred at 100 °C for 3 h in $(CH_2Cl)_2$ under nitrogen atmosphere. The reaction mixture was cooled to room temperatue and diluted with CH_2Cl_2 (30 mL). The organic layer was washed with water (1 x 5 mL) and dried over Na_2SO_4. Evaporation of the solvents gave a resiude that was purified by column chromatography on silica gel using a 1:50 ethyl acetate and hexane. ^{1}H NMR (600 MHZ) analysis showed k_H/k_D = 6.7.



Kinetic Isotope Experiment (Competition)

Parallel kinetic isotope experiment. A mixture of 2-(4-methylphenyl-2,6-d_2)-2*H*-indazole (0.125 mmol), 1,2-diphenylethyne (0.15 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.15 mmol), K_2CO_3 (0.125 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) were charged in $(CH_2Cl)_2$ under nitrogen atmosphere. In another reaction flask 2-(*p*-tolyl)-2*H*-indazole (0.125 mmol), 1,2-diphenylethyne (0.15 mmol), $Cu(OAc)_2 \cdot H_2O$ (0.15 mmol), K_2CO_3 (0.125 mmol) and $[Cp^*RhCl_2]_2$ (4 mol%) were charged in $(CH_2Cl)_2$ under nitrogen atmosphere. These two reaction mixtures was stirred parallely in same preheated oil bath at 100˚ C for 1 hour. These reaction mixtures were combined diluted with CH_2Cl_2 (30 mL). The organic layer was washed with water (1 x 5 mL) and dried over Na_2SO_4. Evaporation of the solvents gave a resiude that was purified by column chromatography on silica gel using a 1:50 ethyl acetate and hexane. ^{1}H NMR (600 MHZ) analysis showed k_H/k_D = 3.8.



Kinetic Isotope Experiment (Parallel)

Crystal Structure of 3h.

We obtained a green crystal of **3h** grown from slow evaporation technique using 2:1 mixture of dichloromethane and acetonitrile. This crystal suited for single-crystal X-ray diffraction study, other crystallographic details see table. The ORTEP diagram clearly indicated that indazolo[2,3-a]quinoline ring is coplanar geometry and two aryl rings are orthogonal. The angle between phenyl ring and indazolo[2,3-a]quinoline ring are observed to be 123.04° (C17-C8-C9) and 121.42° (C8-C9-C-23). The crystal packing shows that head to tail arrangement according to reduce the dipole-dipole interaction. Further, we observed π-π interaction of two antiparallel pair with 3.349 Å interplanar distance. Structural information was deposited at the Cambridge Crystallographic Data Center (CCDC 1817425).

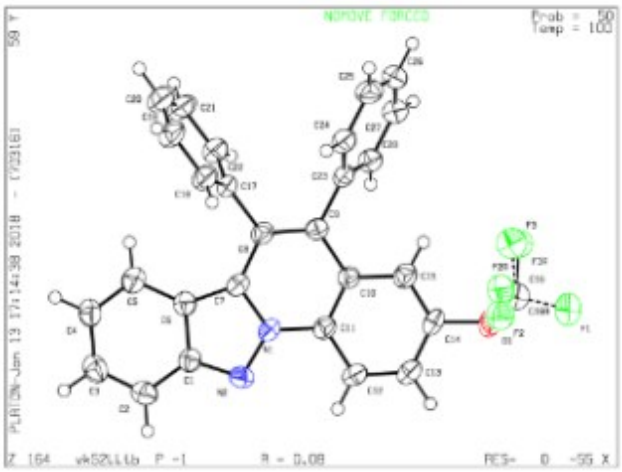


Figure 1. ORTEP diagram of **3h** (thermal elipsoids drawn at the 30% probability level)

Identification code	vk52iitb
Empirical formula	$C_{28}H_{17}F_3N_2O$
Formula weight	454.59
Temperature(K)	100.15
Radiation	MoKα (λ = 0.71073)
Crystal system	triclinic
Space group	P-1
a/Å	7.9330(6)
b/Å	11.1848(7)
c/Å	13.1762(10)
a /°	72.919(6)
b /°	73.841(6)
γ/°	84.499(5)
V/ Å^3	1073.27(14)
Crystal size(mm^3)	0.164 × 0.07 × 0.04
Z	2
Density(Mg /m^{-3})	1.407
Final R[I>2s(I)]	R_1 = 0.0827, wR_2 = 0.1973
R(all data)	R_1 = 0.1282, wR_2 = 0.2309
Collected reflns	21709
Unique reflns	3751 [R_{int} = 0.1169, R_{sigma} = 0.0832]
Theta range for data collection	5.514 to 49.996
Absorption coefficient(mm^{-1})	0.104
Goodness of fit on F^2	1.051
CCDC No.	1817425

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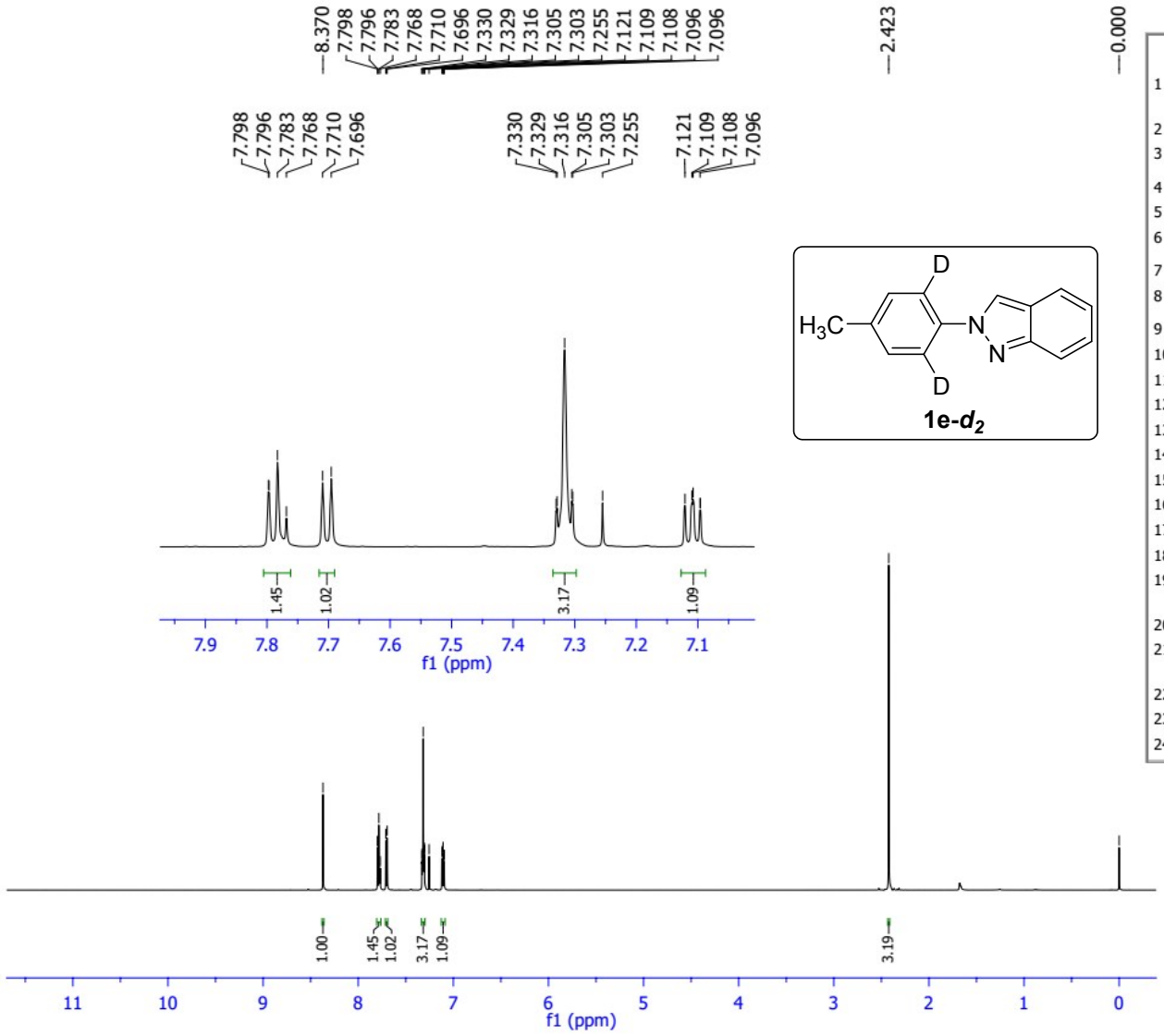
^{1}H and ^{13}C NMR spectra



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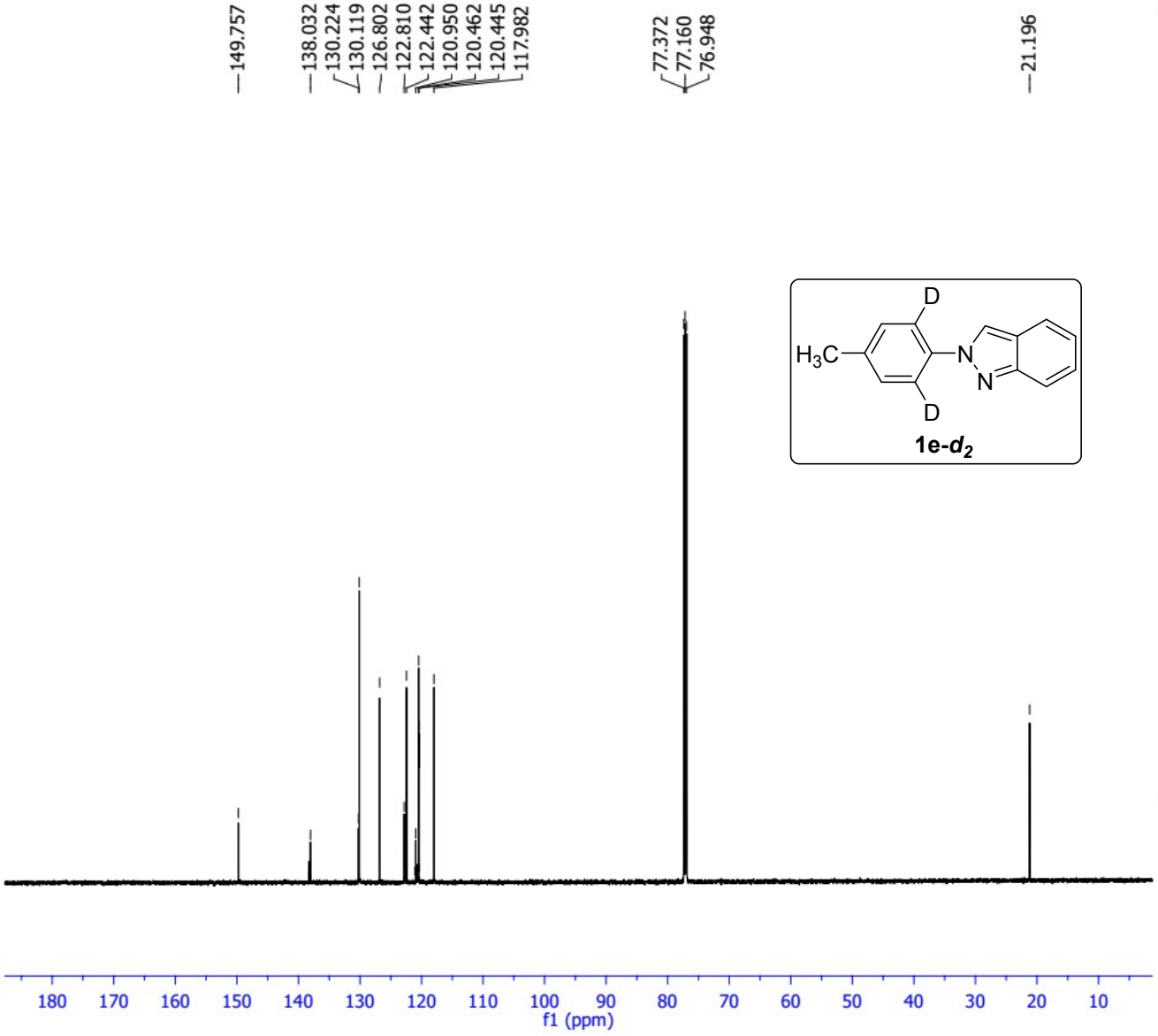

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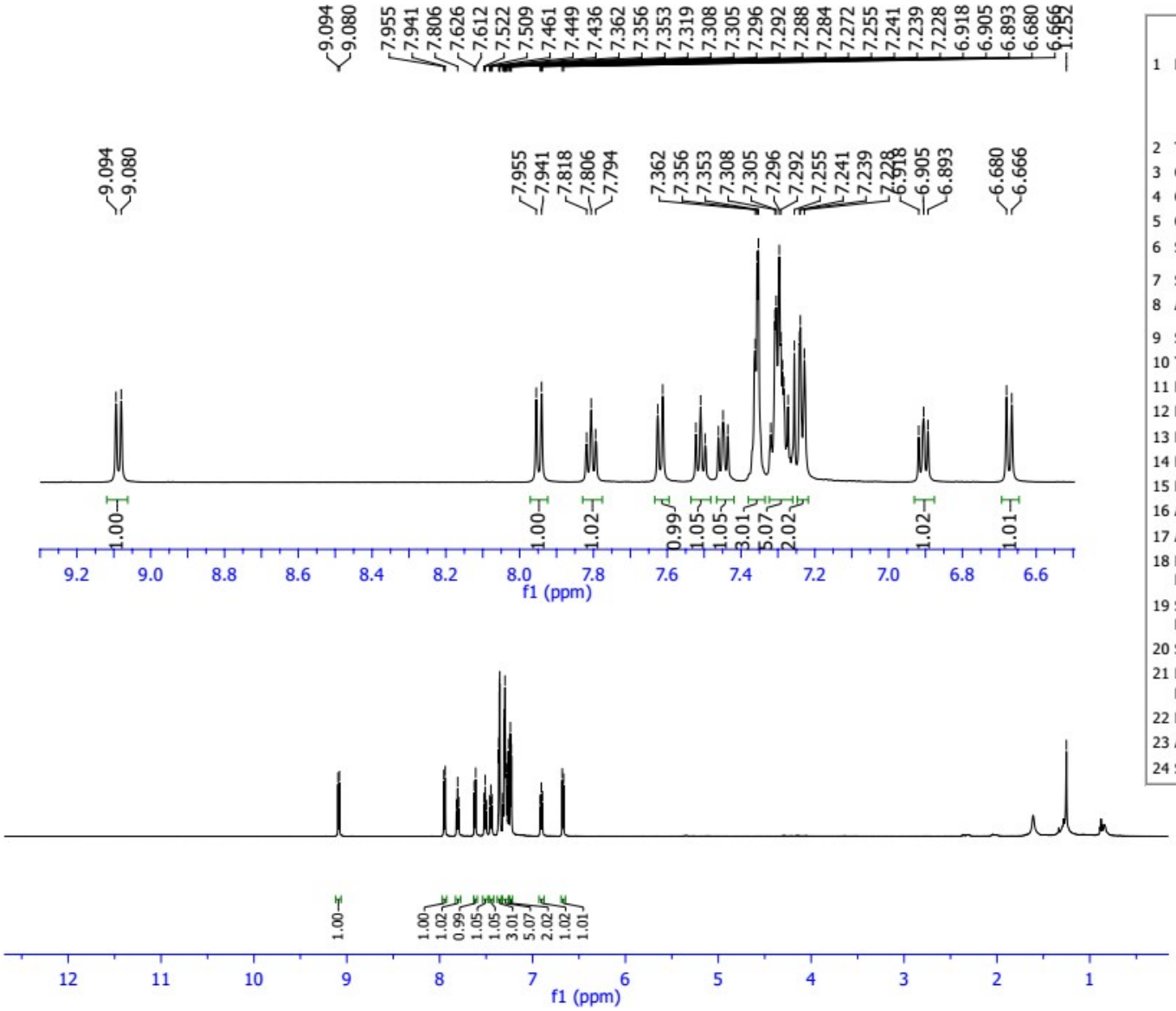

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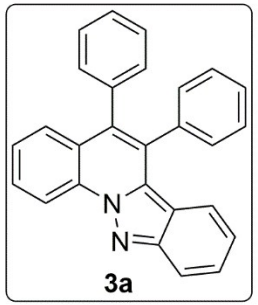
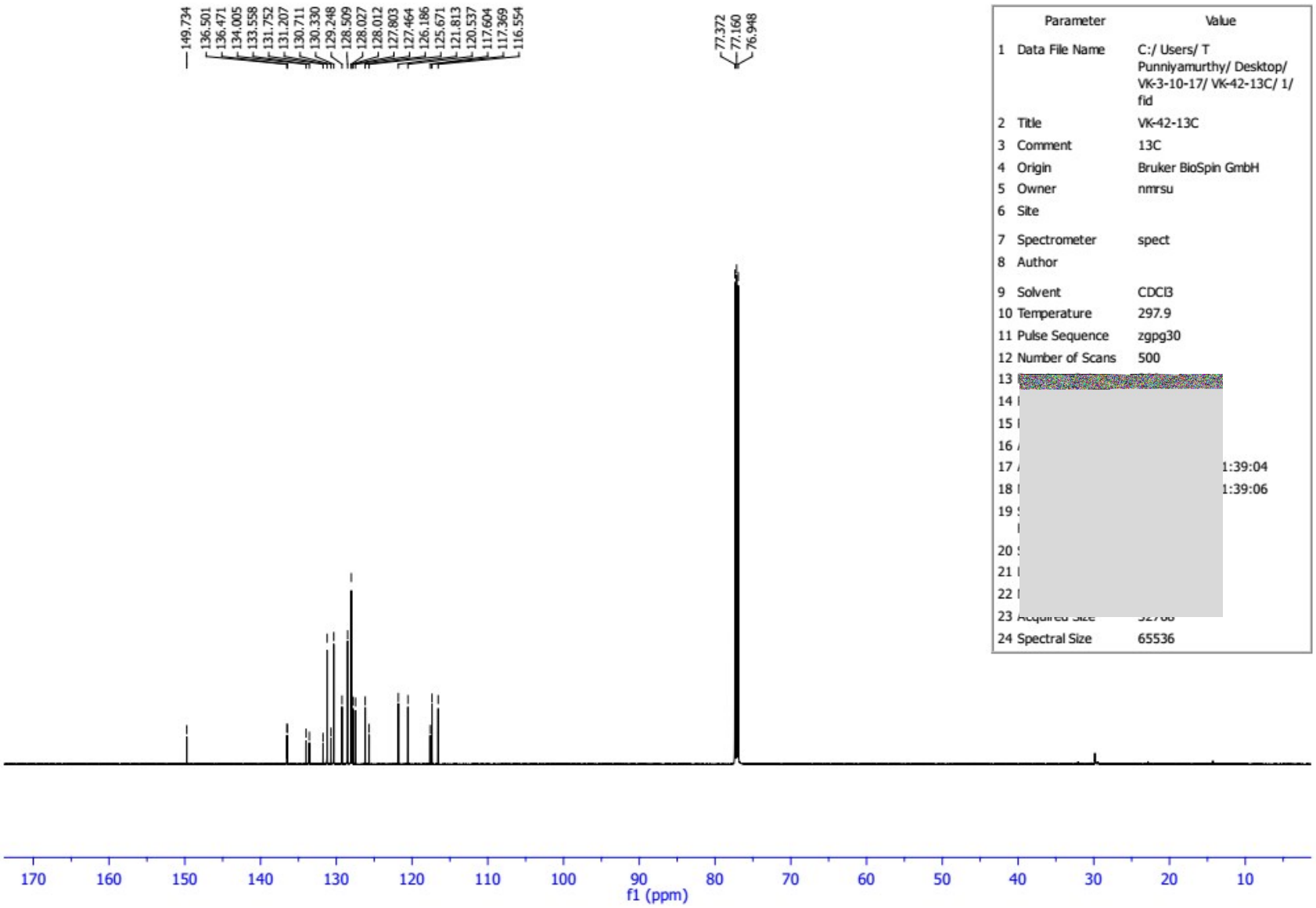


3a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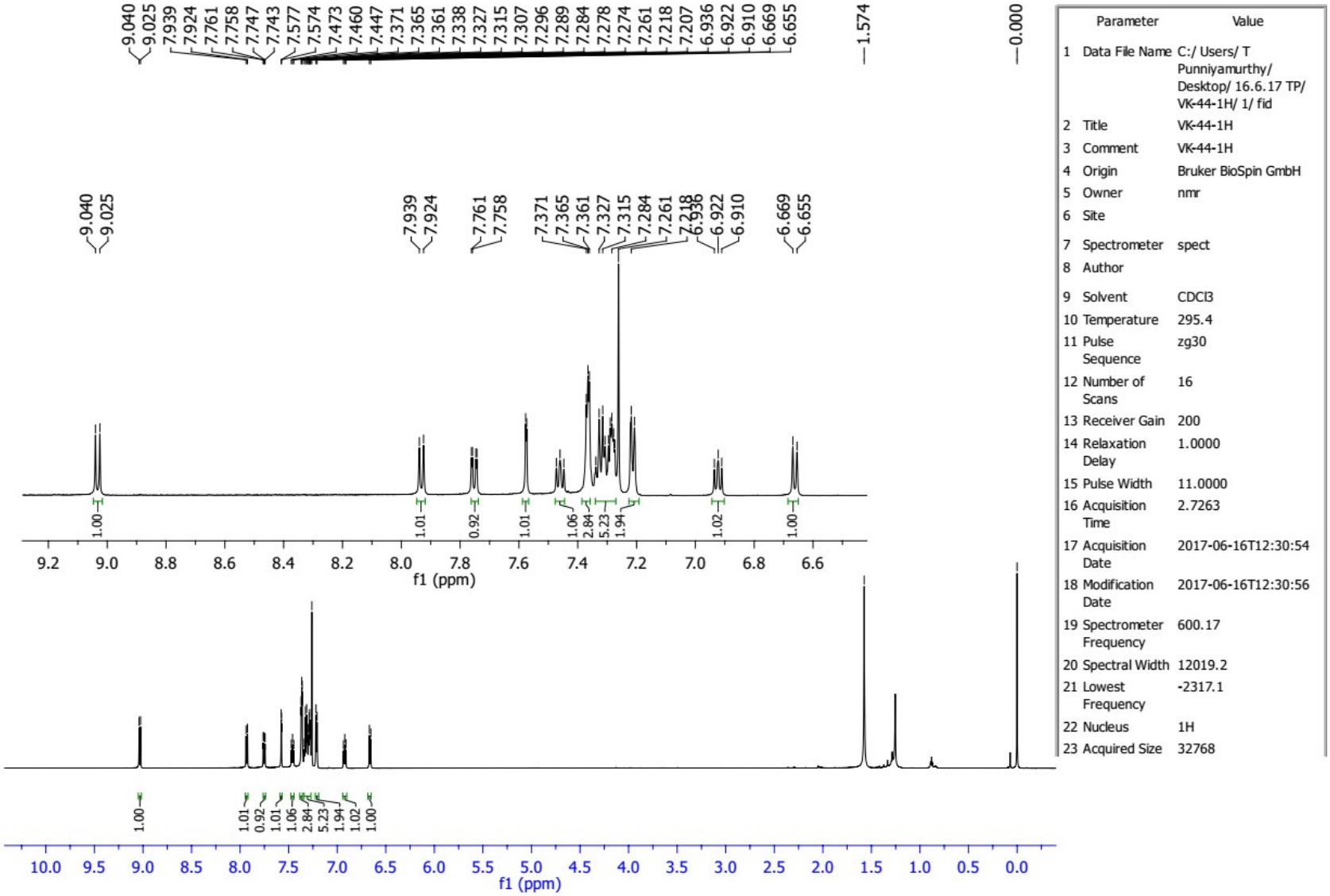

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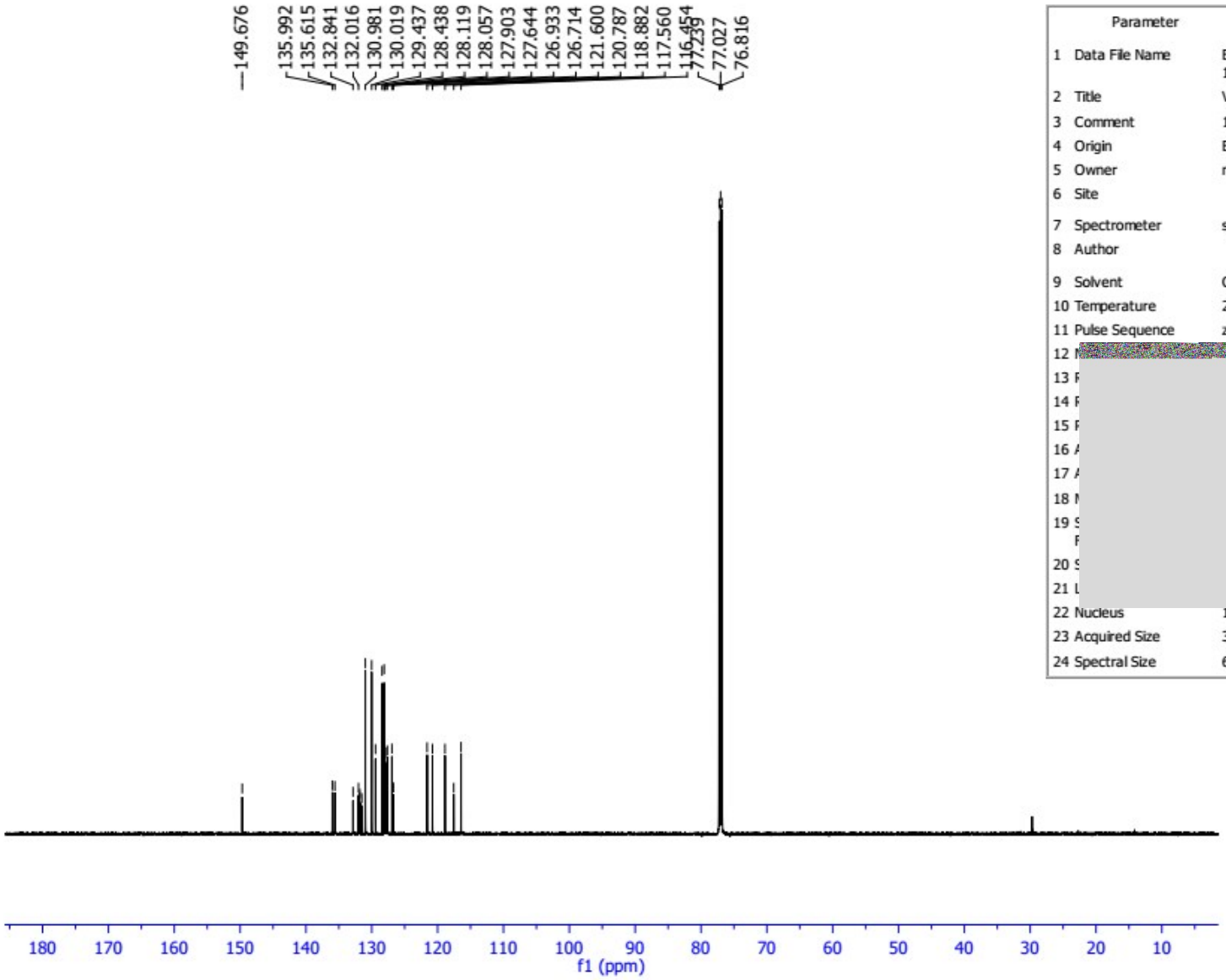

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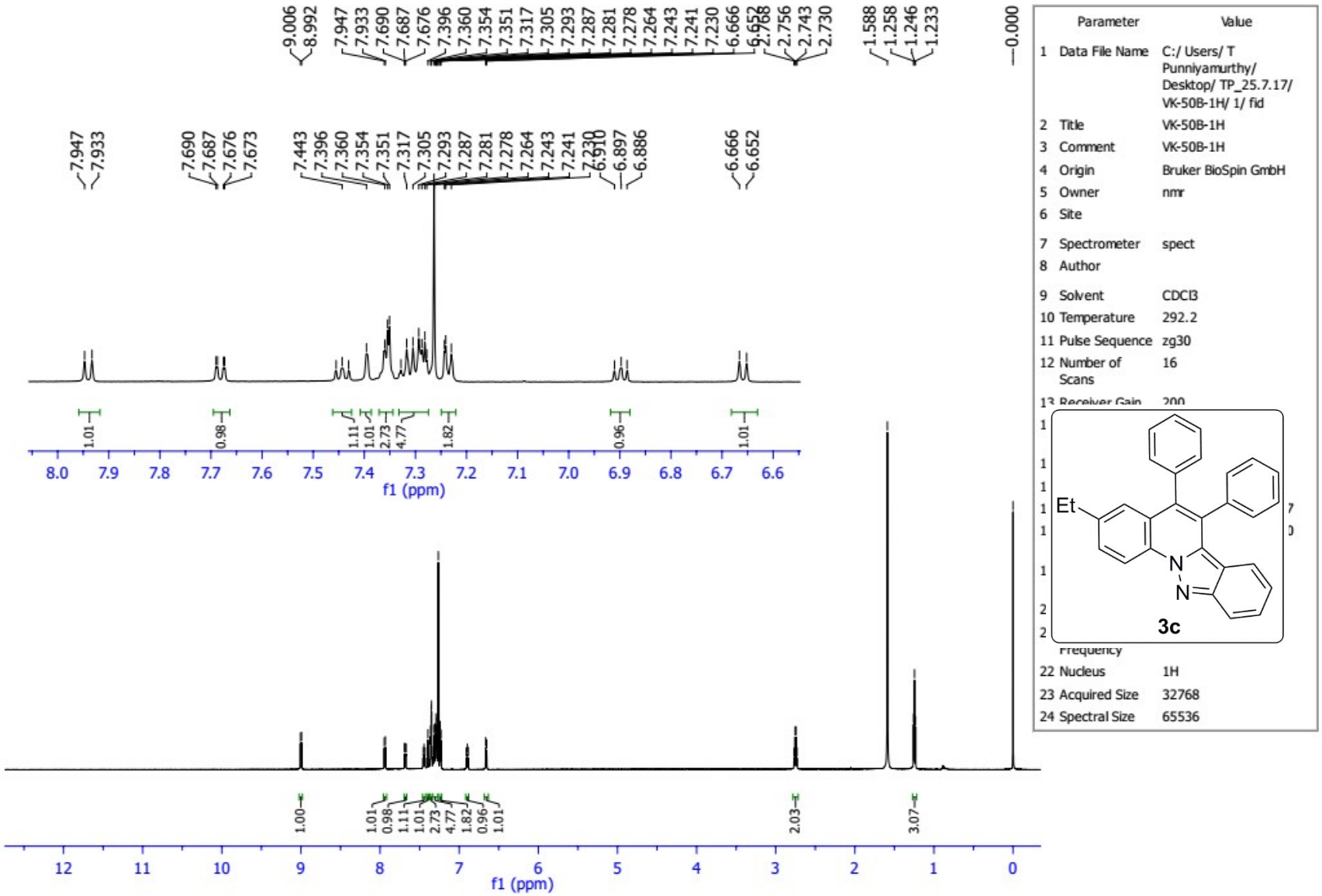
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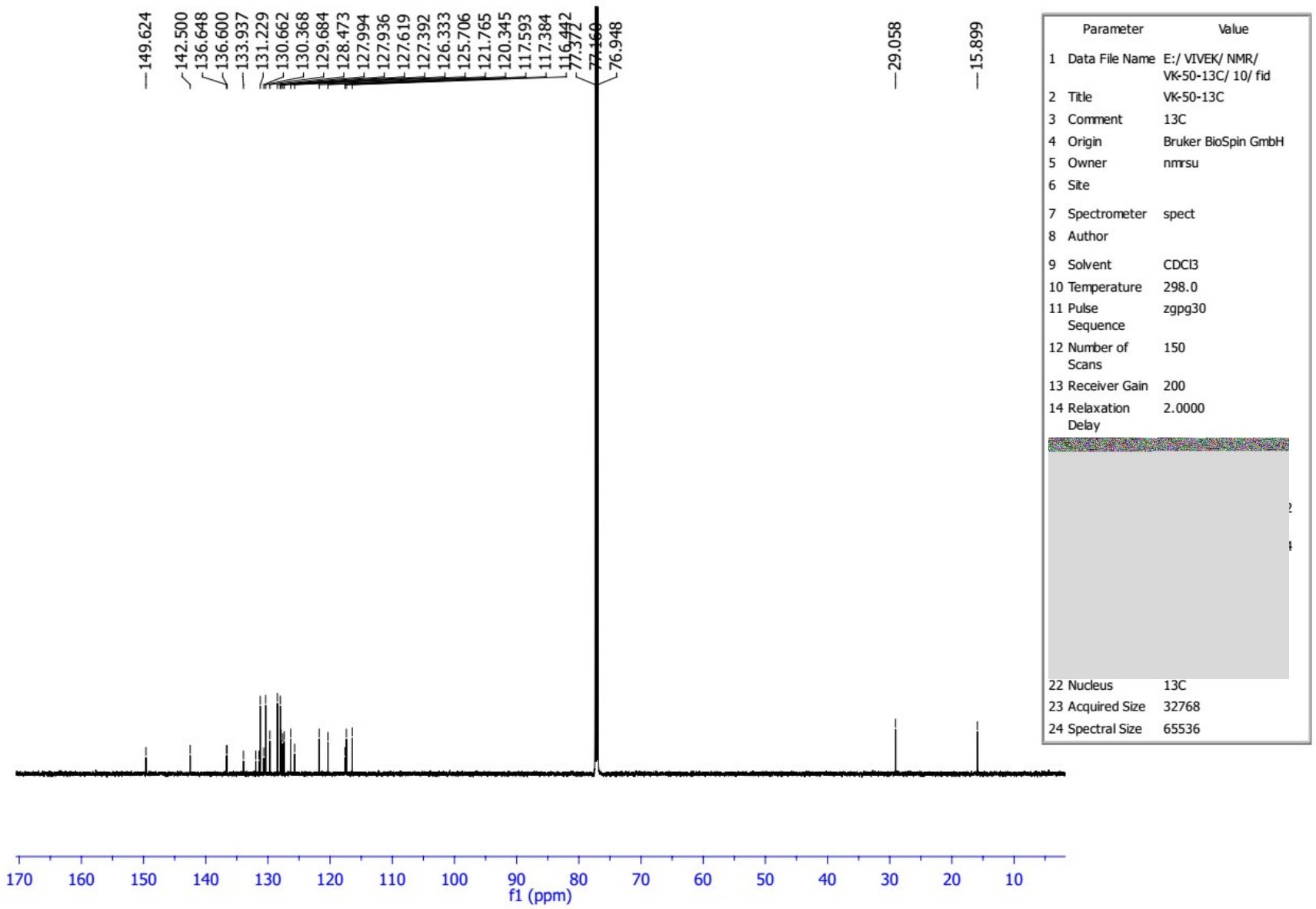
24 Spectral Size
65536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136.648
136.600
133.937
131.229
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130.368
129.684
128.473
127.994
127.936
127.619
127.392
126.333
125.706
121.765
120.345
117.593
117.384
116.442
77.372
77.160
76.948
29.058
15.899
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Value
1 Data File Name E:/ VIVEK/ NMR/ VK-50-13C/ 10/ fid
2 Title VK-50-13C
3 Comment 13C
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence zgpg30
12 Number of Scans 150
13 Receiver Gain 200
14 Relaxation Delay 2.0000
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536
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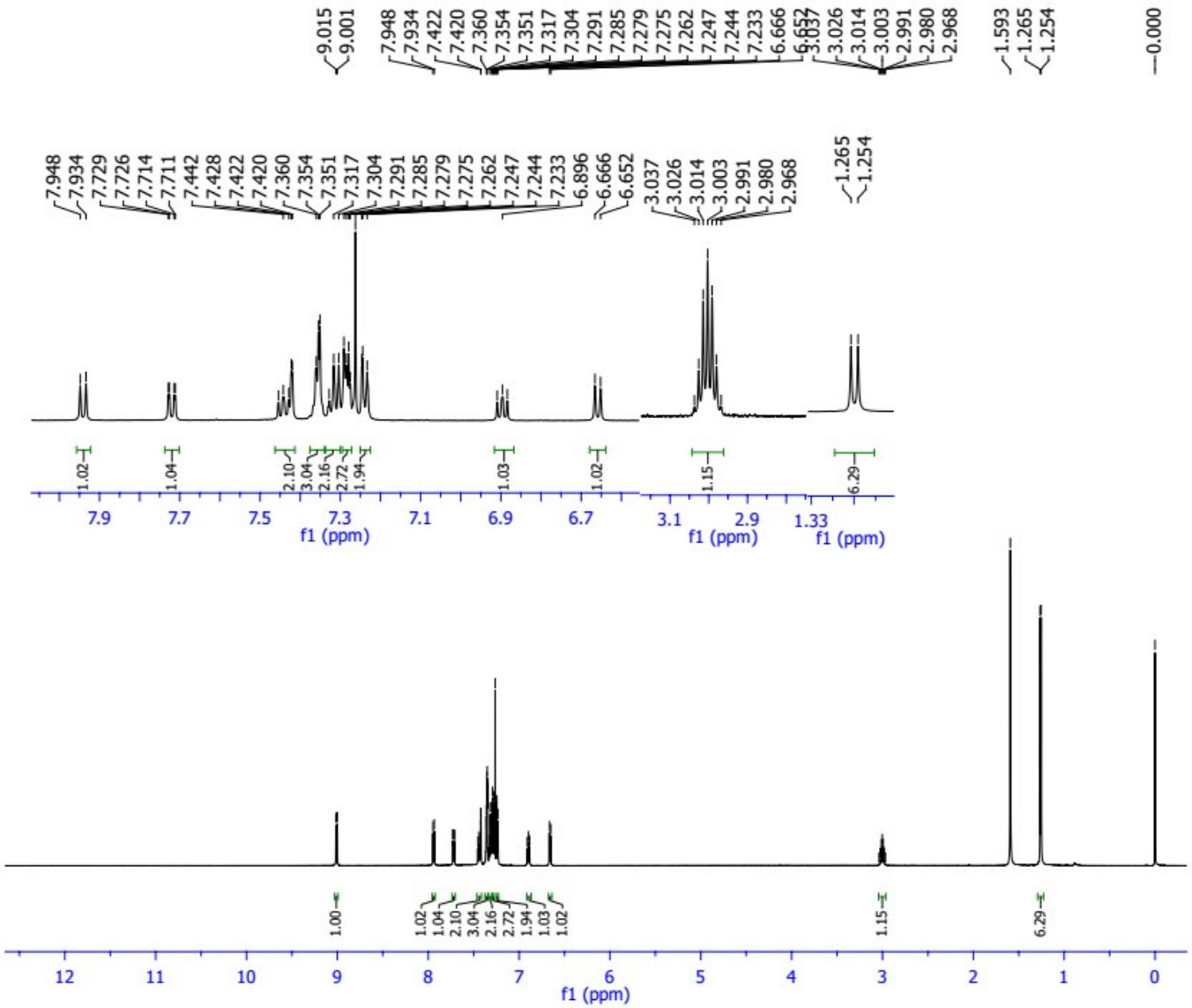
f1 (ppm)



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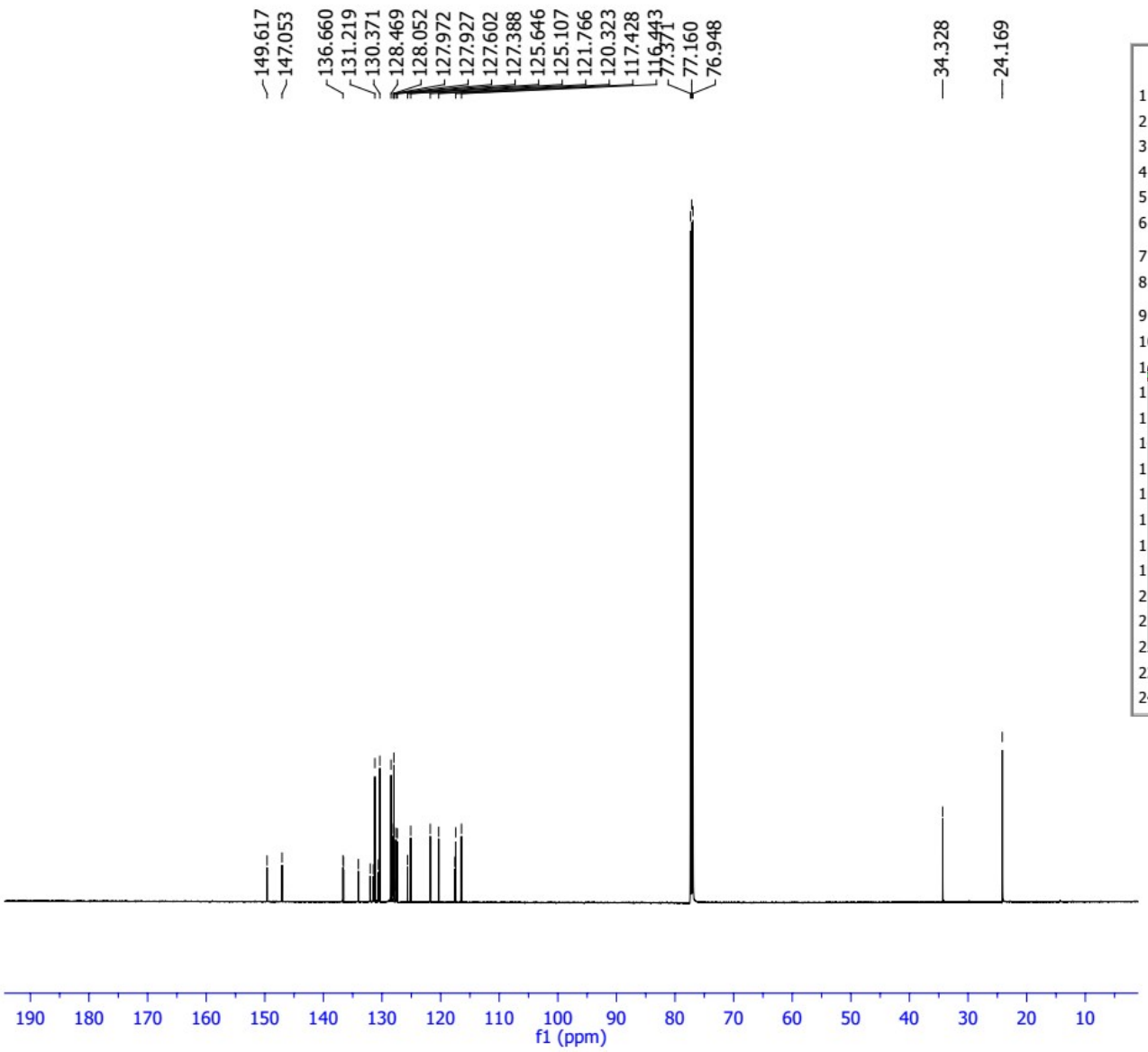
2	Title	VK-51-1H
3	Comment	VK-51-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	200
14	Relaxation Delay	1.0000
15	Pulse Width	11.0000
16	Acquisition Time	2.7263
17	Acquisition Date	2017-07-25T16:16:41
18	Modification Date	2017-07-25T16:16:44
19	Spectrometer Frequency	600.17
20	Spectral Width	12019.2
21	Lowest Frequency	-2316.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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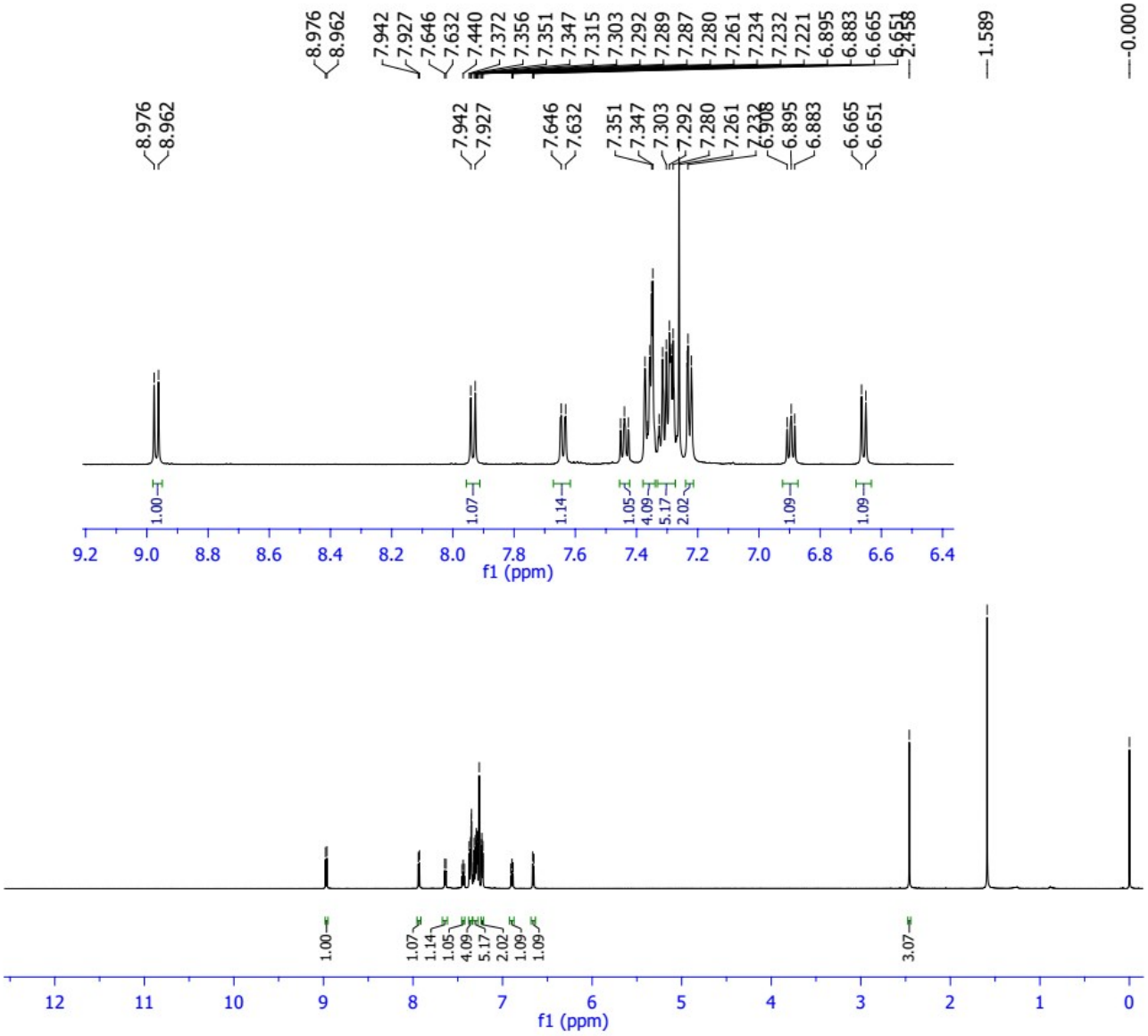
2	Title	VK-51-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
23	Acquired Size	32768
24	Spectral Size	65536



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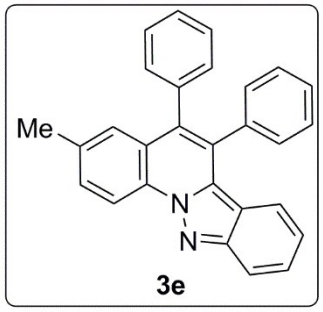
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK 20-06-17/ VK-45-1H/ 10/ fid
2	Title	VK-45-1H
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.6
	Frequency	
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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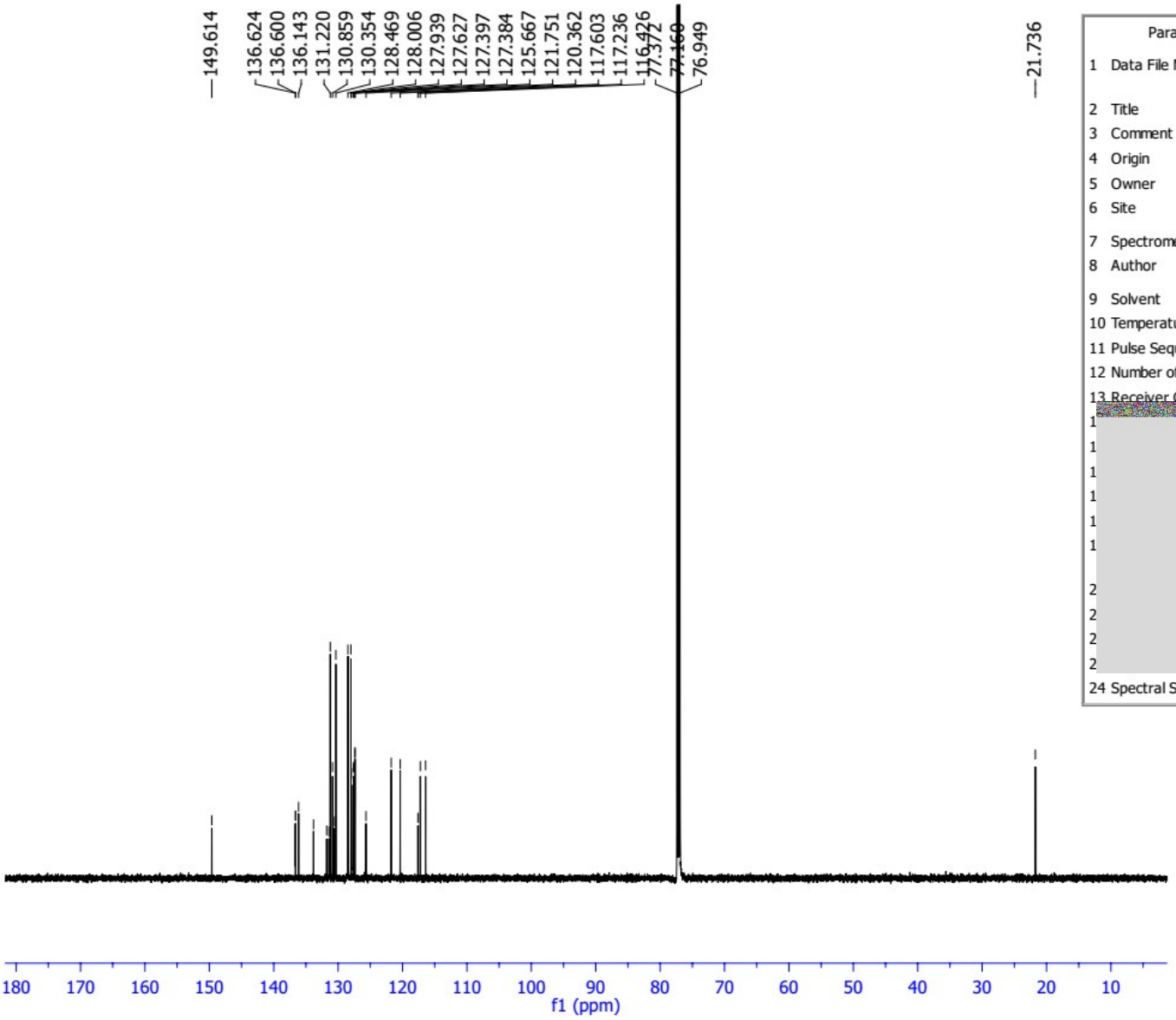

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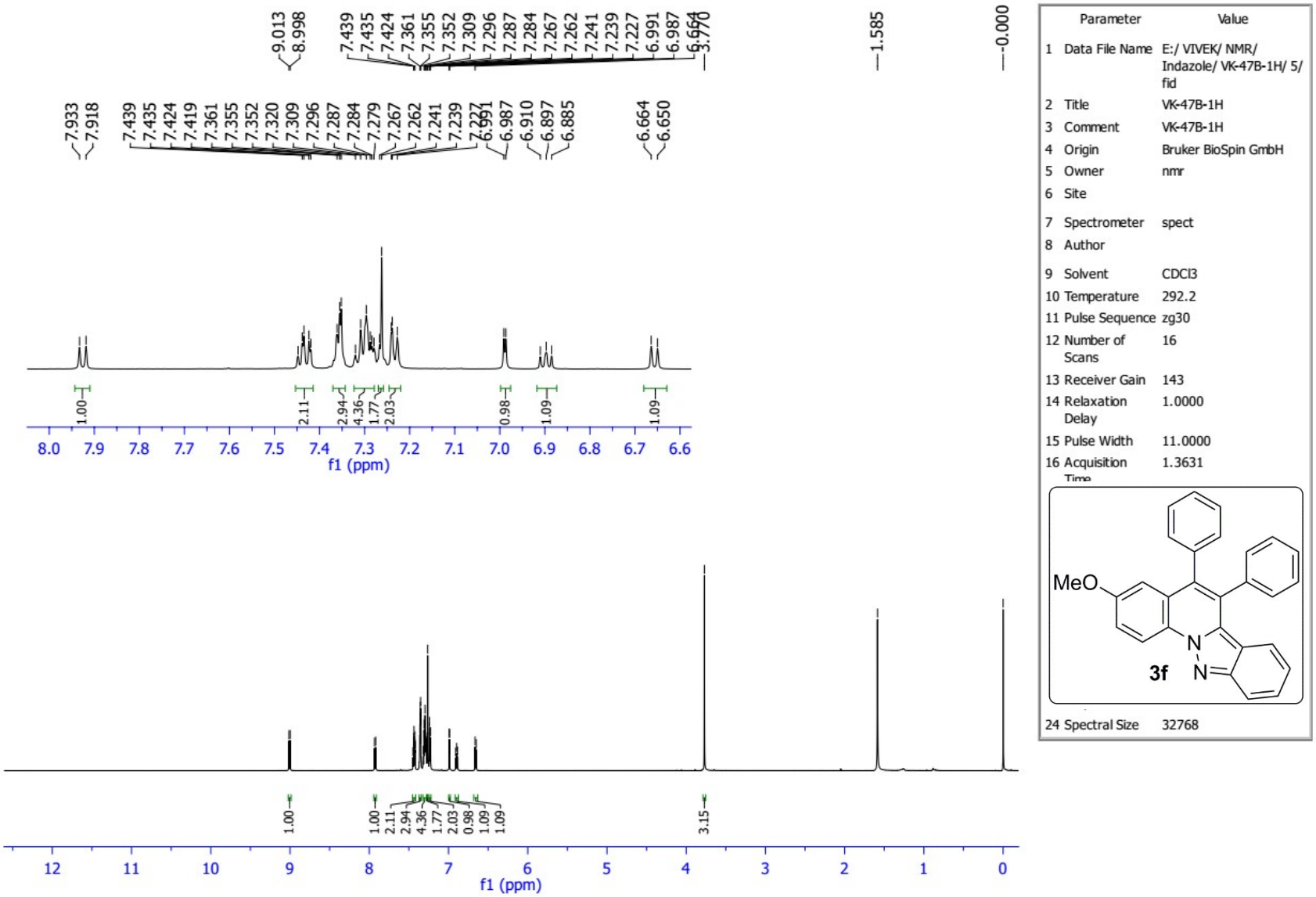
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	150
13	Receiver Gain	200
24	Spectral Size	65536



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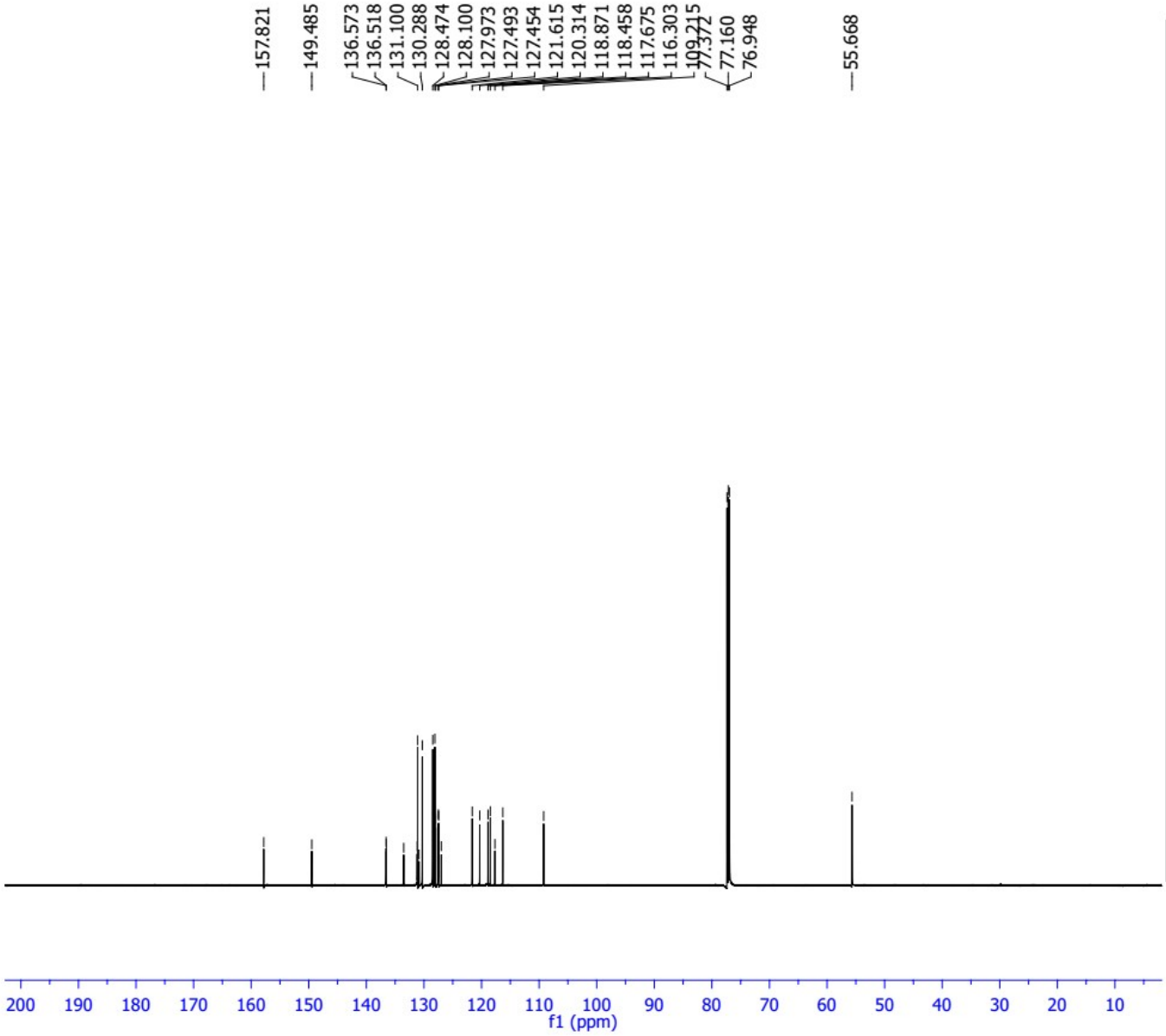
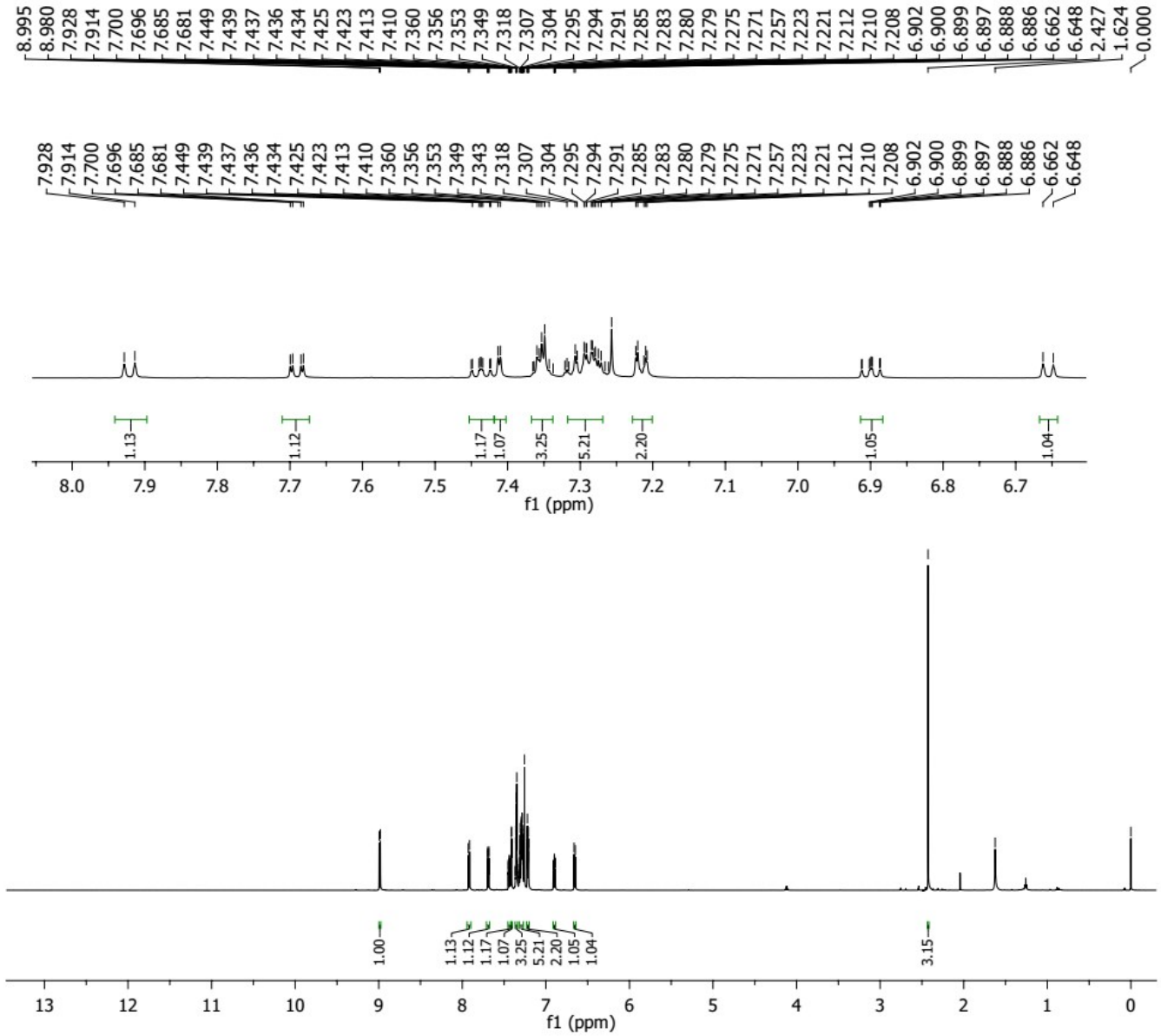
2	Title	VK-47B-1H
3	Comment	VK-47B-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	143
14	Relaxation Delay	1.0000
15	Pulse Width	11.0000
16	Acquisition Time	1.3631

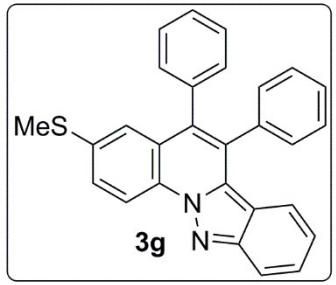
24	Spectral Size	32768

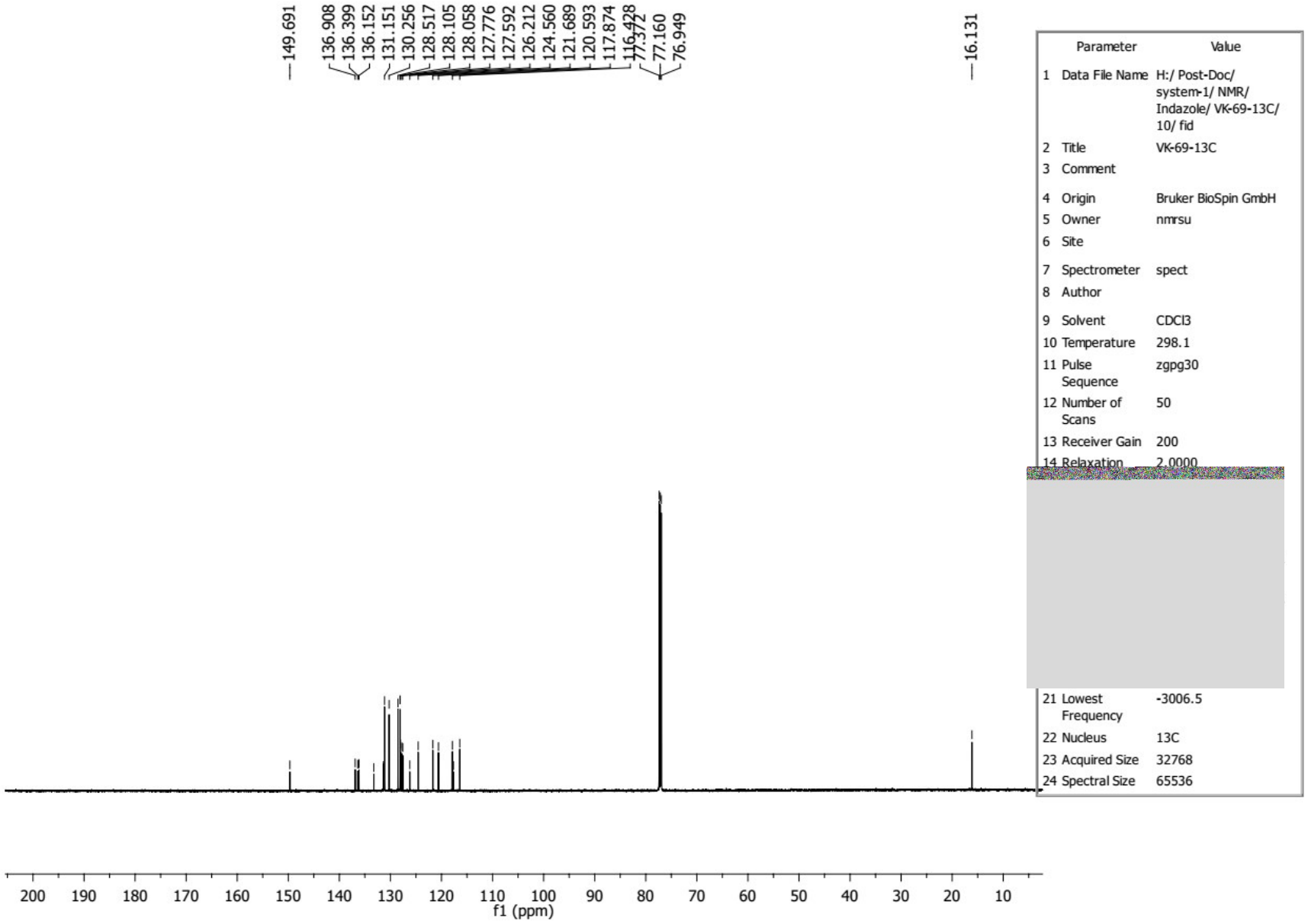


	Parameter	Value
1	Data File Name	H:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-47-13C/ 10/ fid
2	Title	VK-47-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	150
13	Receiver Gain	200
14	Relaxation Delay	2.0000
15	Pulse Width	12.0000
23	Acquired Size	32768
24	Spectral Size	65536

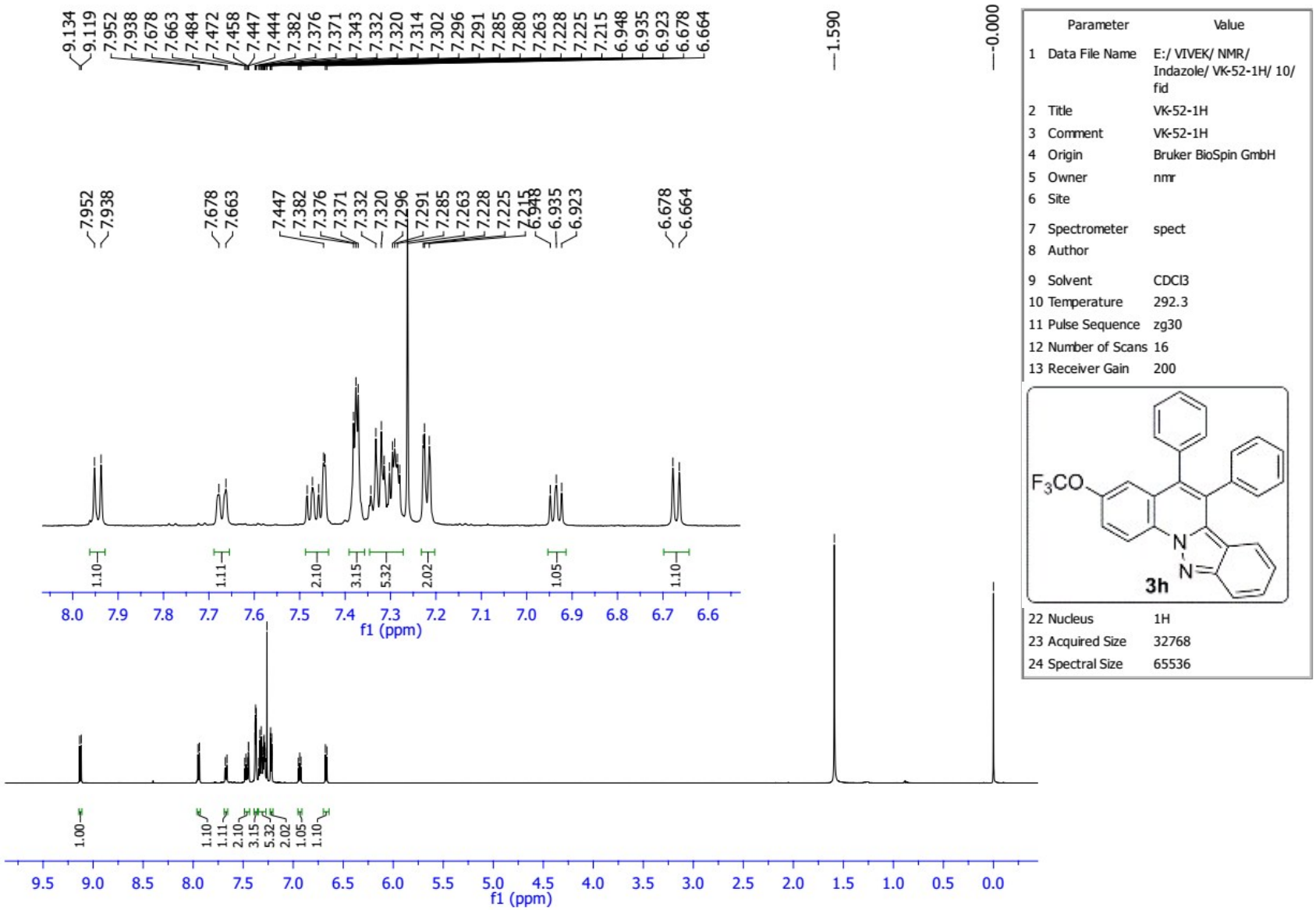


	Parameter	Value
1	Data File Name	H:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-69-1H/ 10/ fid
2	Title	VK-69-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	10
14	Relaxation Delay	1.0000
15	Pulse Width	7.5500
23	Acquired Size	32768
24	Spectral Size	65536





	Parameter	Value
1	Data File Name	H:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-69-13C/ 10/ fid
2	Title	VK-69-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Number of Scans	50
13	Receiver Gain	200
14	Relaxation	2.0000
21	Lowest Frequency	-3006.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536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7.472
7.458
7.447
7.444
7.382
7.376
7.371
7.343
7.332
7.320
7.314
7.302
7.296
7.291
7.285
7.280
7.263
7.228
7.225
7.215
6.948
6.935
6.923
6.678
6.664
1.590
0.000
1.10
1.11
2.10
3.15
5.32
2.02
1.05
1.10
f1 (ppm)
1.00
1.10
1.11
2.10
3.15
5.32
2.02
1.05
1.10
f1 (ppm)
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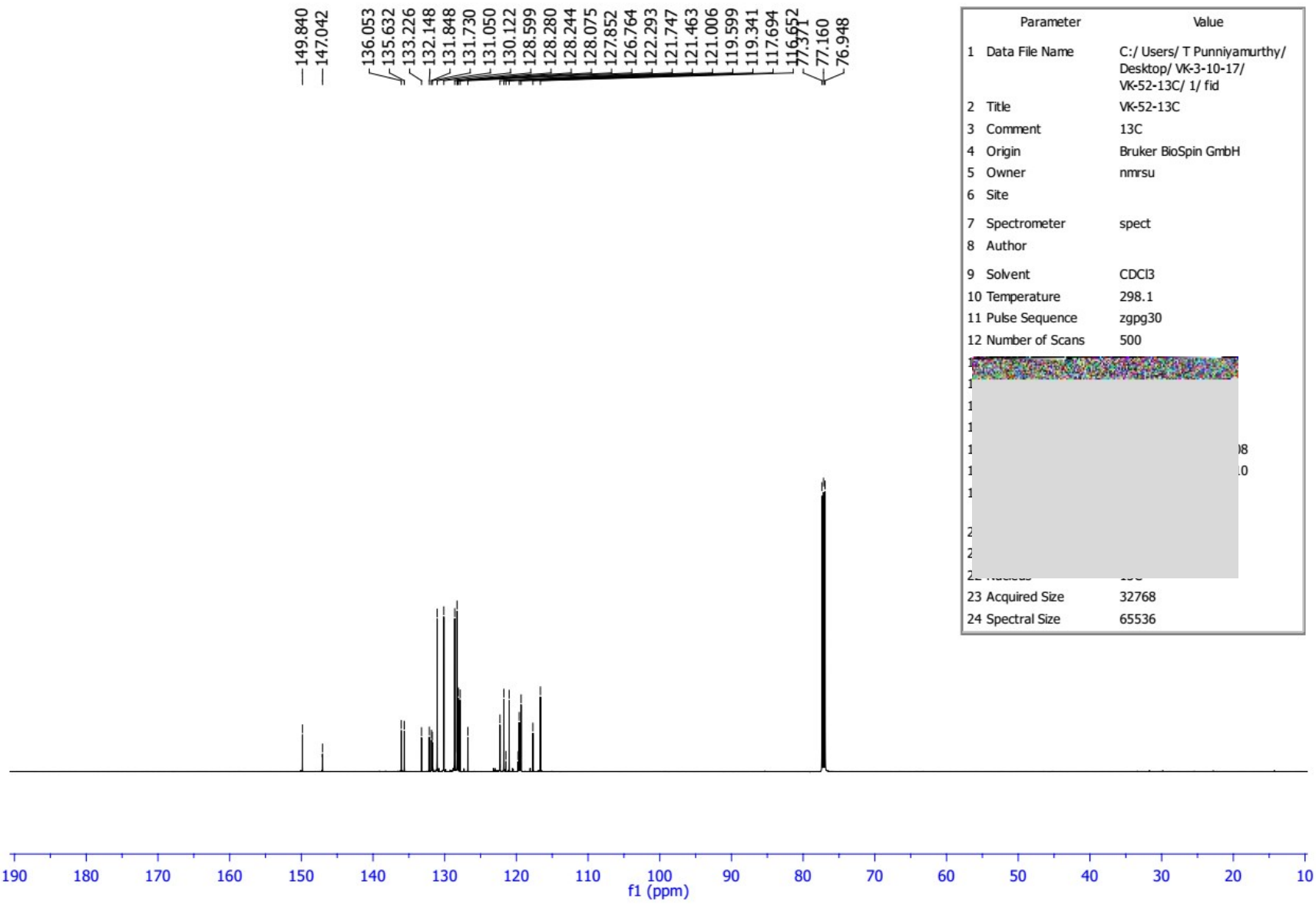
2 Title VK-52-1H
3 Comment VK-52-1H
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 292.3
11 Pulse Sequence zg30
12 Number of Scans 16
13 Receiver Gain 200
F3CO
N
N
3h
22 Nucleus 1H
23 Acquired Size 32768
24 Spectral Size 65536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132.148
131.848
131.730
131.050
130.122
128.599
128.280
128.244
128.075
127.852
126.764
122.293
121.747
121.463
121.006
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119.341
117.694
116.652
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77.160
76.948
Parameter
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2 Title
VK-52-13C
3 Comment
13C
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
298.1
11 Pulse Sequence
zgpg30
12 Number of Scans
500
23 Acquired Size
32768
24 Spectral Size
65536
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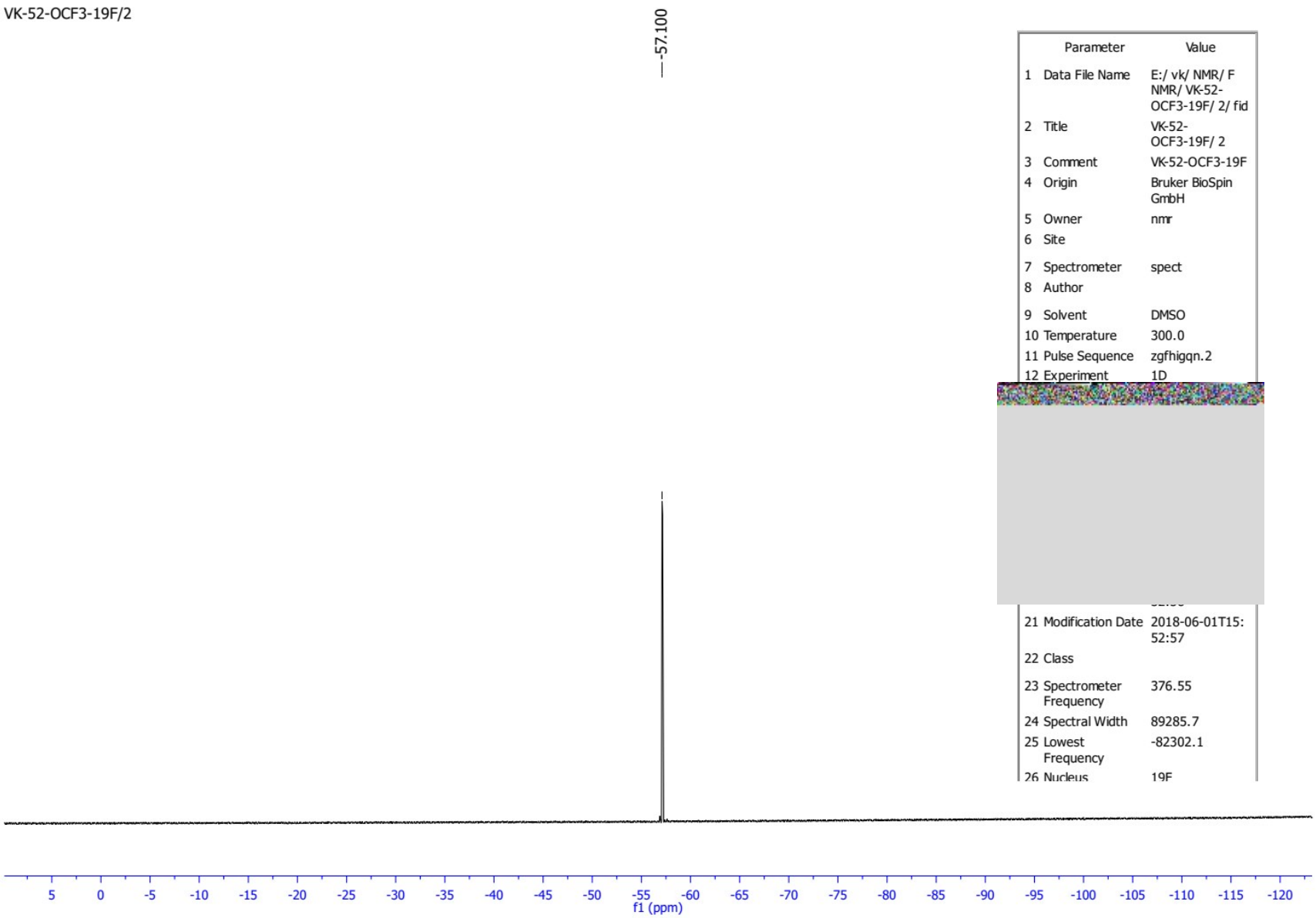
f1 (ppm)


VK-52-OCF3-19F/2
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Parameter Value
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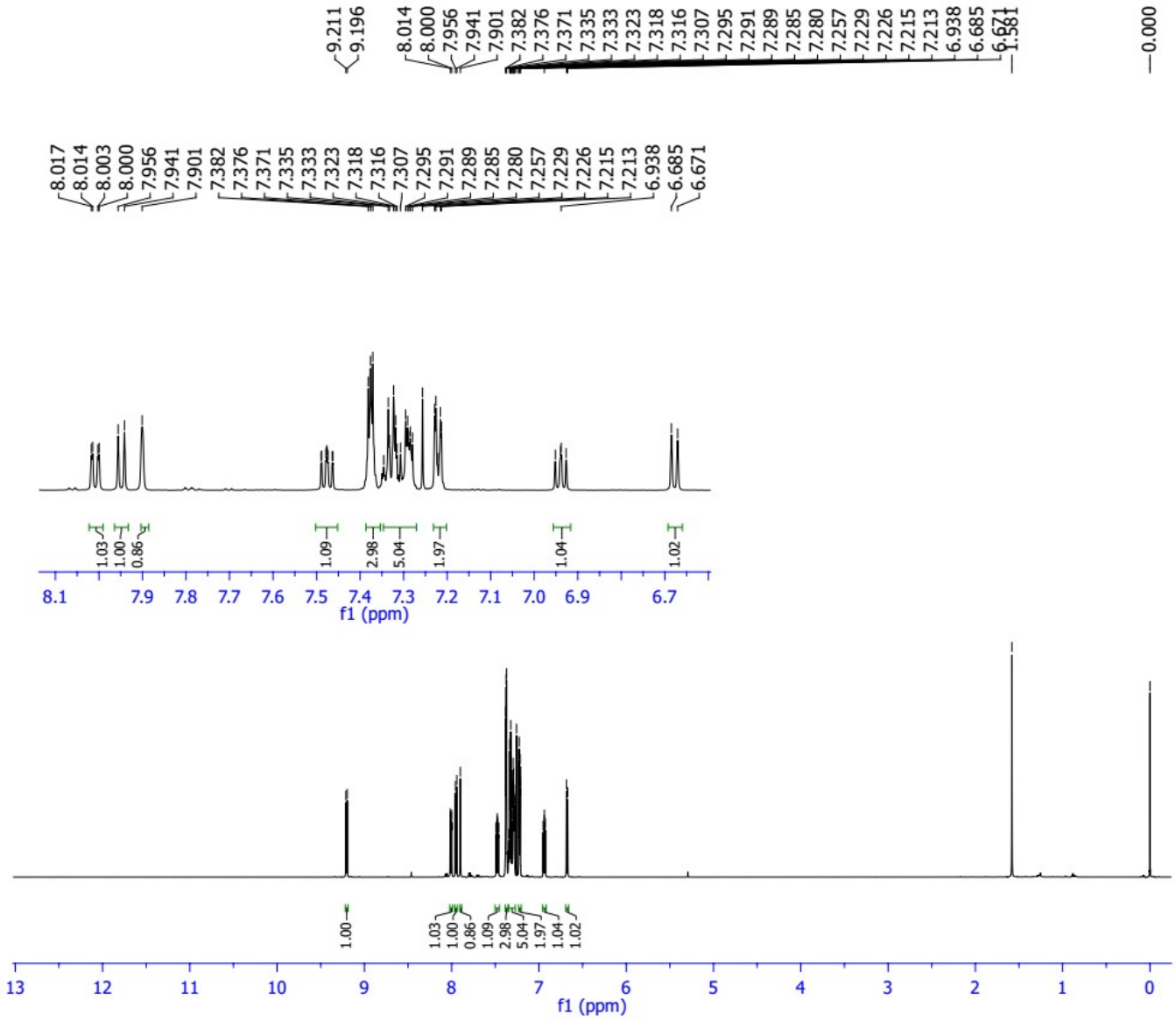
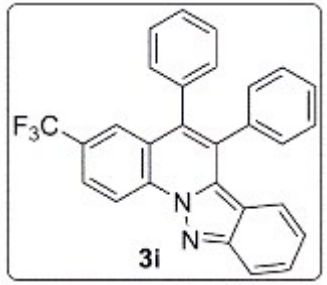
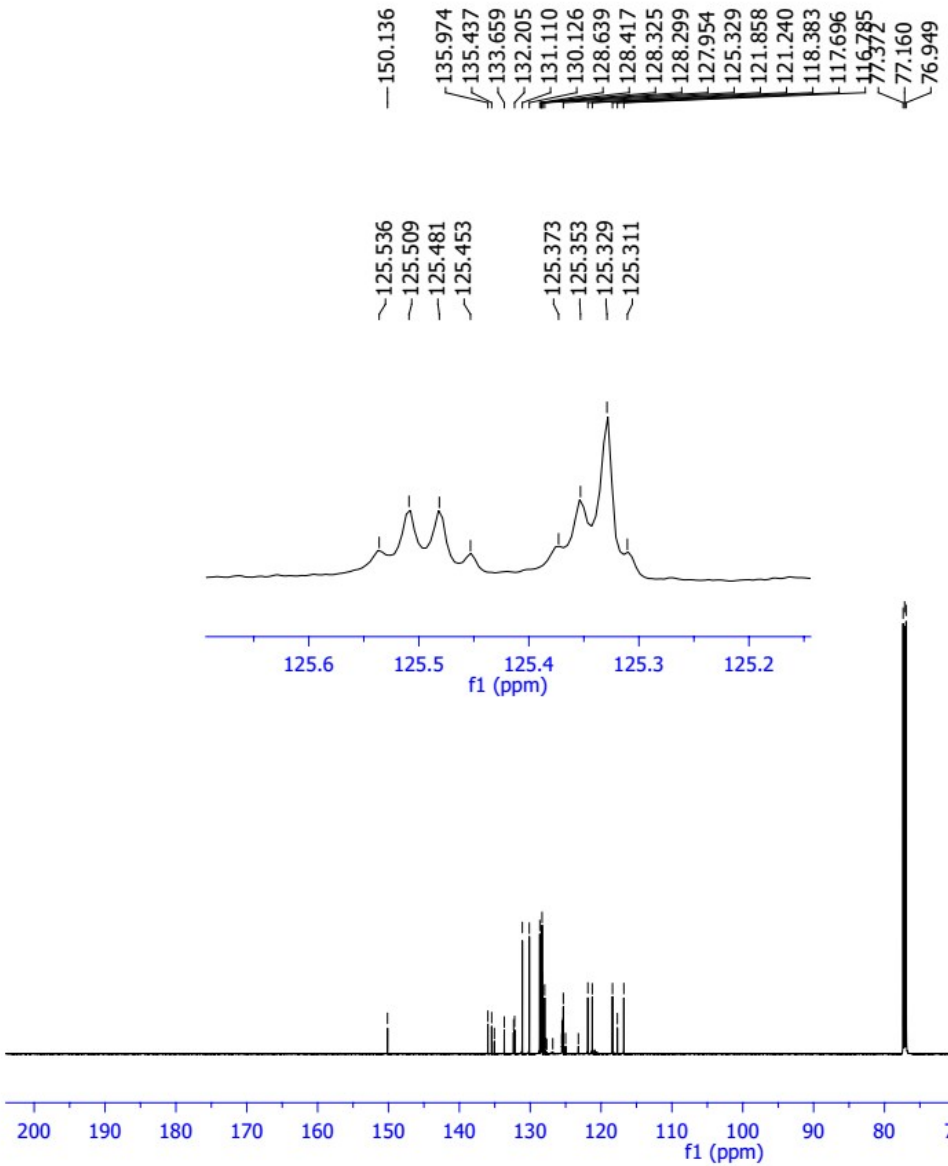
2 Title VK-52-OCF3-19F/ 2
3 Comment VK-52-OCF3-19F
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent DMSO
10 Temperature 300.0
11 Pulse Sequence zgfhigqn.2
12 Experiment 1D
21 Modification Date 2018-06-01T15:52:57
22 Class
23 Spectrometer Frequency 376.55
24 Spectral Width 89285.7
25 Lowest Frequency -82302.1
26 Nucleus 19F
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120
f1 (ppm)



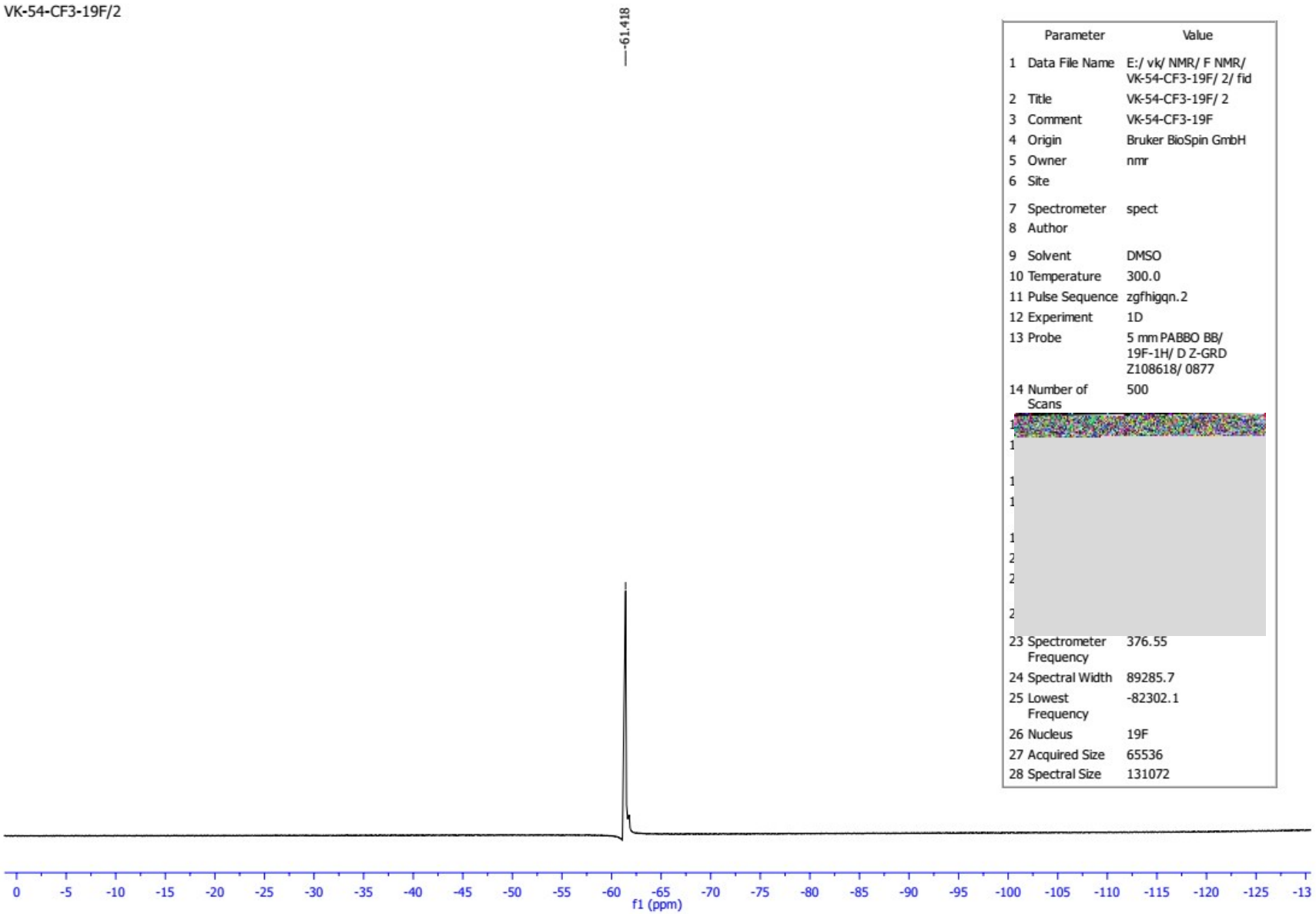
	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ SV-VK-DM-27-09-17/ VK-54A-1H/ 10/ fid
2	Title	VK-54A-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	10
14	Relaxation	1.0000
21	Lowest Frequency	-2321.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536





	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ SV-VK-DM-27-09-17/ VK-54A-13C/ 10/ fid
2	Title	VK-54A-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	500
13	Receiver Gain	200
24	Spectral Size	65536

VK-54-CF3-19F/2



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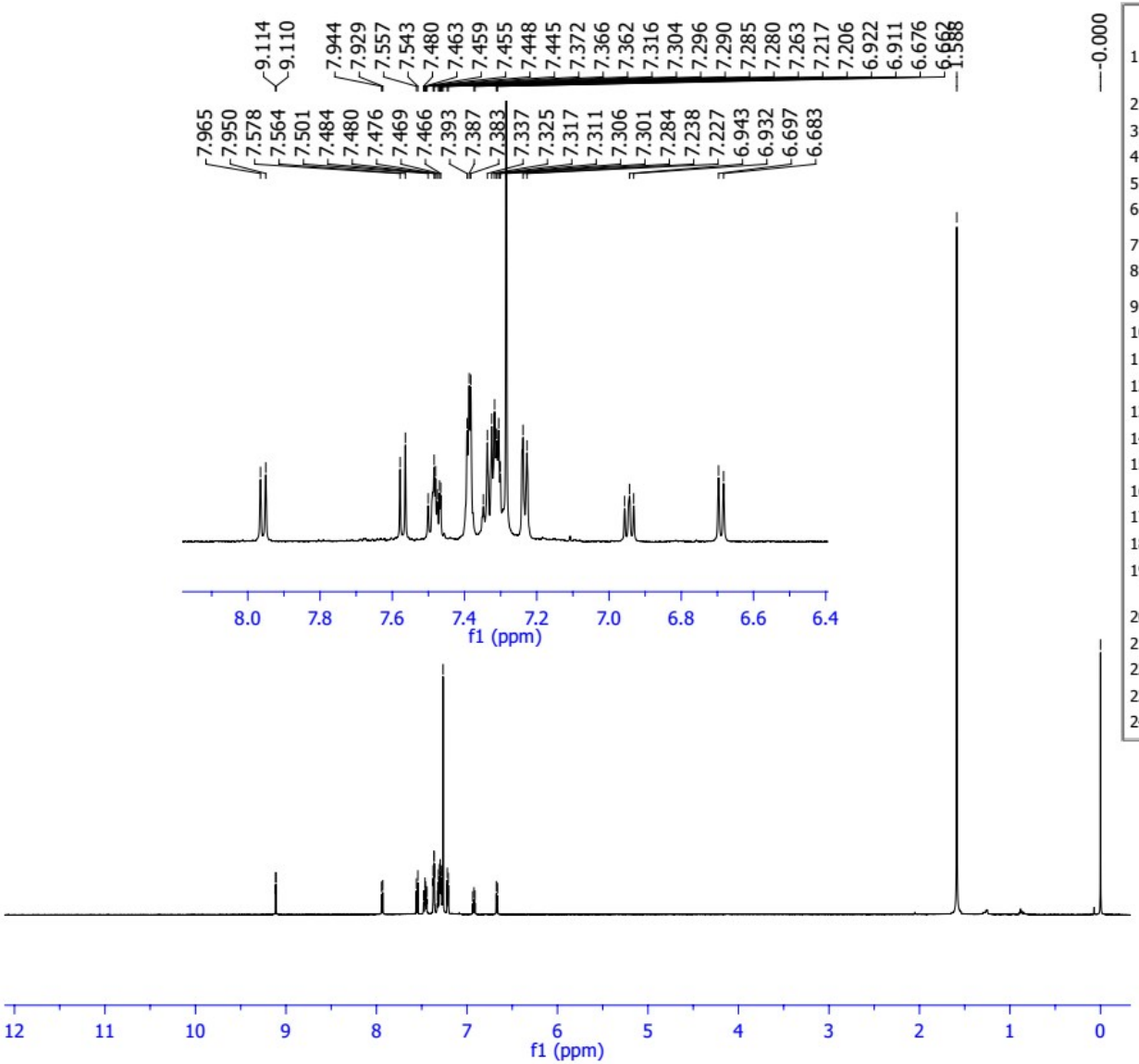
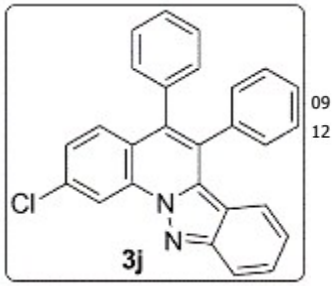
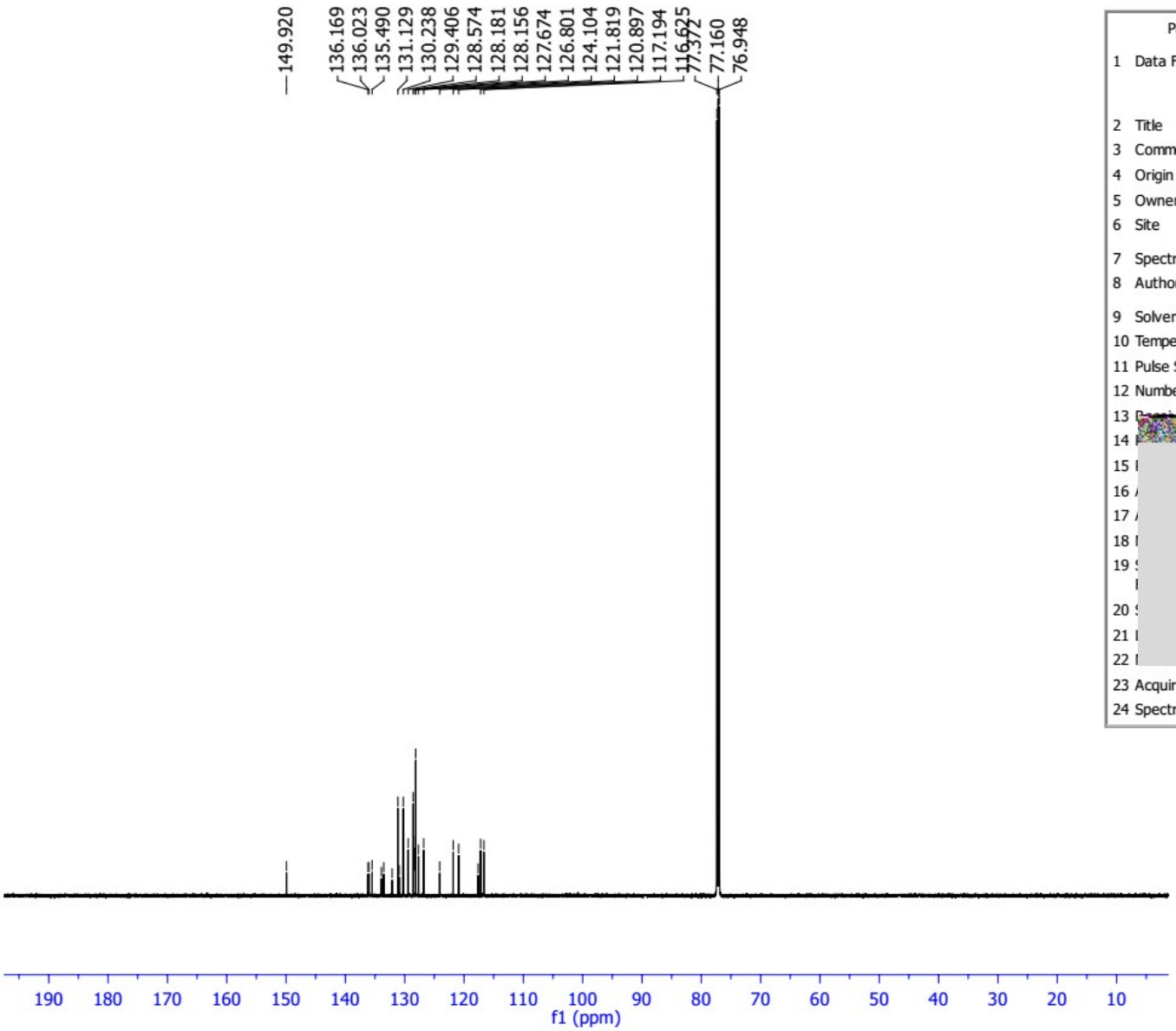
3	Comment	VK-54-CF3-19F
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgfhigqn.2
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0877
14	Number of Scans	500
23	Spectrometer Frequency	376.55
24	Spectral Width	89285.7
25	Lowest Frequency	-82302.1
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072



	Parameter	Value
1	Data File Name	G:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-56-1H/ 10/ fid
2	Title	VK-56-1H
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	200
14	Rel	
15	Pul	
16	Acc	
17	Acc	
18	Mo	
19	Spe Fre	
20	Spe	
21	Low	
22	Nuc	
23	Acquired Size	32768
24	Spectral Size	65536



09
12



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1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-TP-25-9-17/ VK-56-13C/ 10/ fid
2	Title	VK-56-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Number of Scans	100
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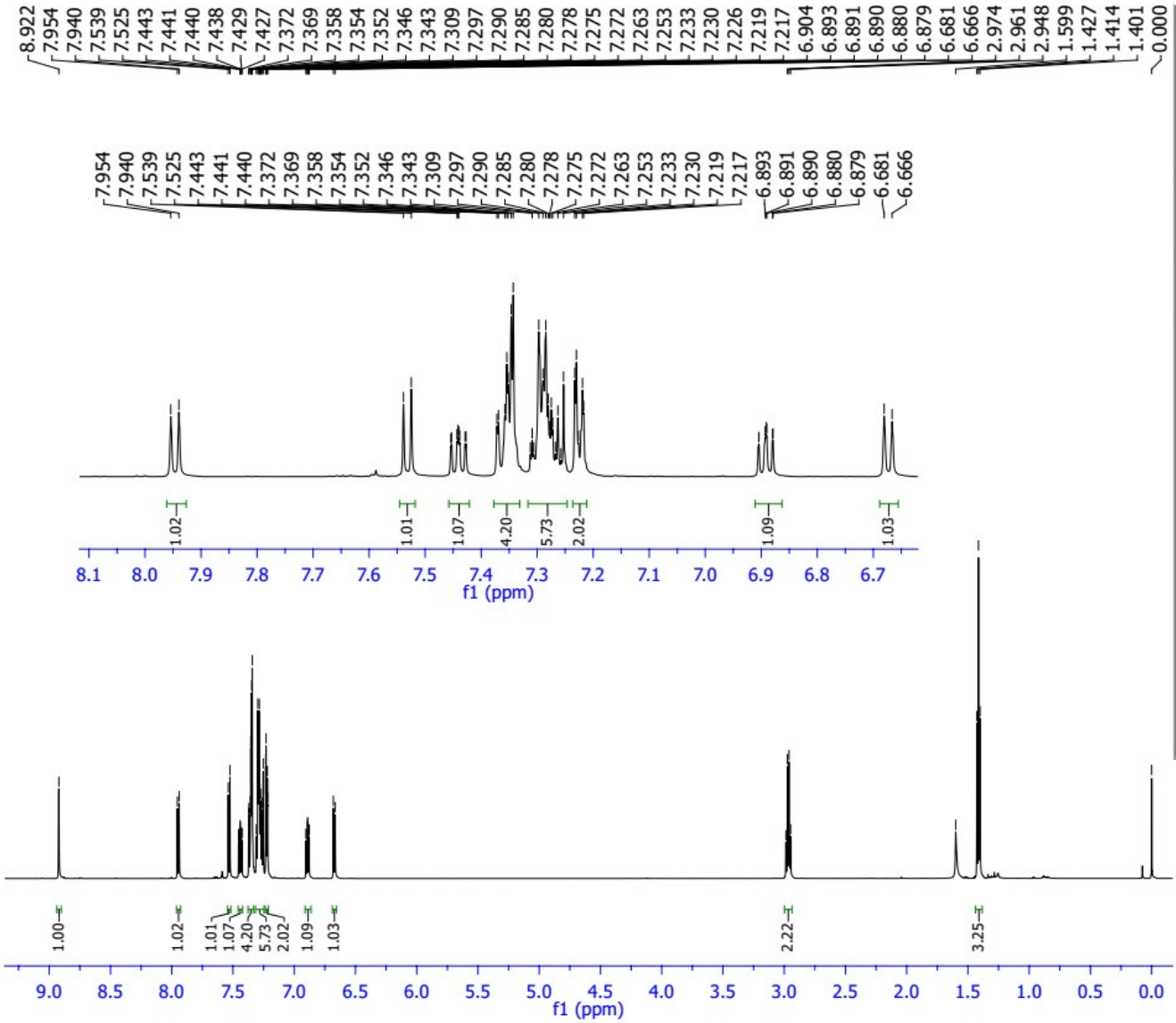
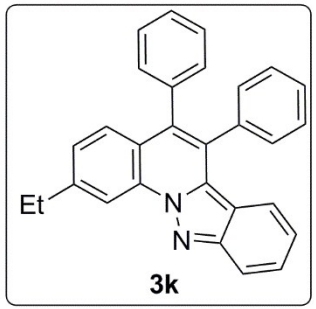
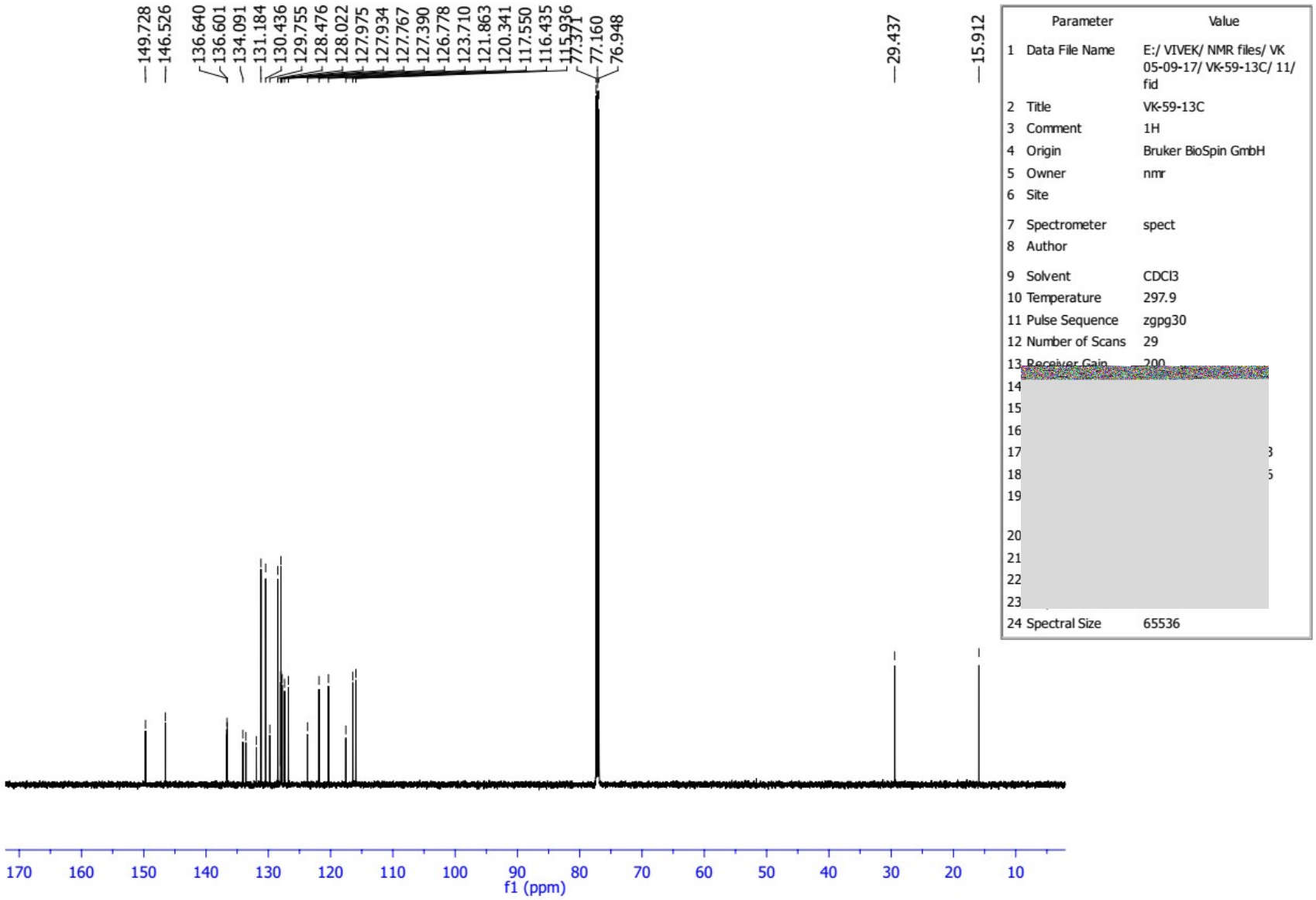
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ VIVEK/ NMR files/ VK 05-09-17/ VK-59-1H/ 10/ fid
2	Title	VK-59-1H
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12	Number of Scans	8
13–21		
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

3k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126.778
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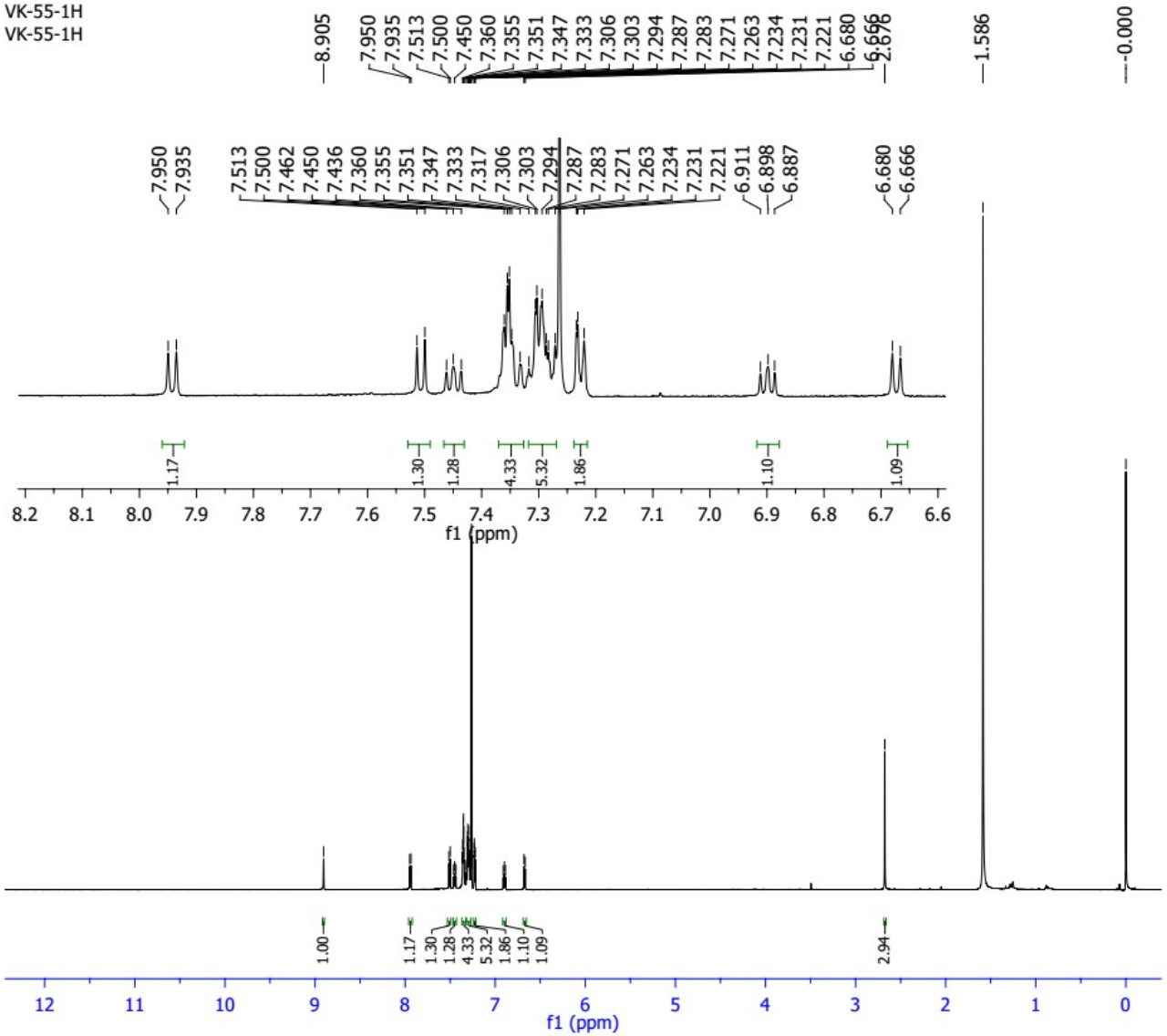
121.863
120.341
117.550
116.435
115.936
77.371
77.160
76.948
29.437
15.912
Parameter
Value
1 Data File Name
E:/ VIVEK/ NMR files/ VK 05-09-17/ VK-59-13C/ 11/ fid
2 Title
VK-59-13C
3 Comment
1H
4 Origin
Bruker BioSpin GmbH
5 Owner
nmr
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
297.9
11 Pulse Sequence
zgpg30
12 Number of Scans
29
13 Receiver Gain
200
24 Spectral Size
65536
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



	Parameter	Value
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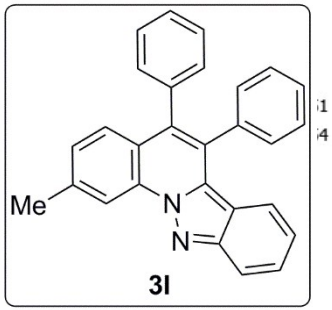
2	Title	VK-55-1H
3	Comment	VK-55-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.1
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	200



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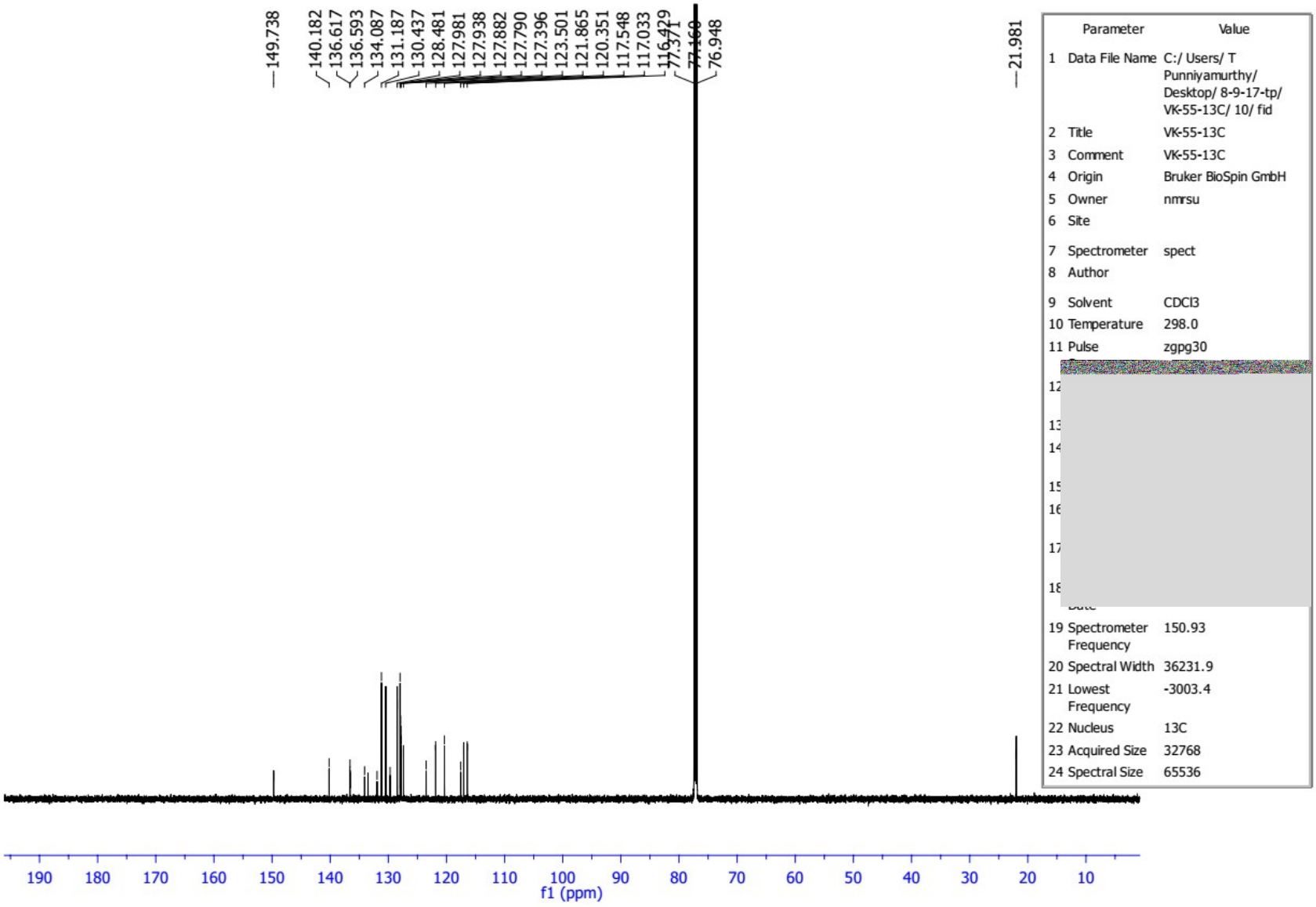
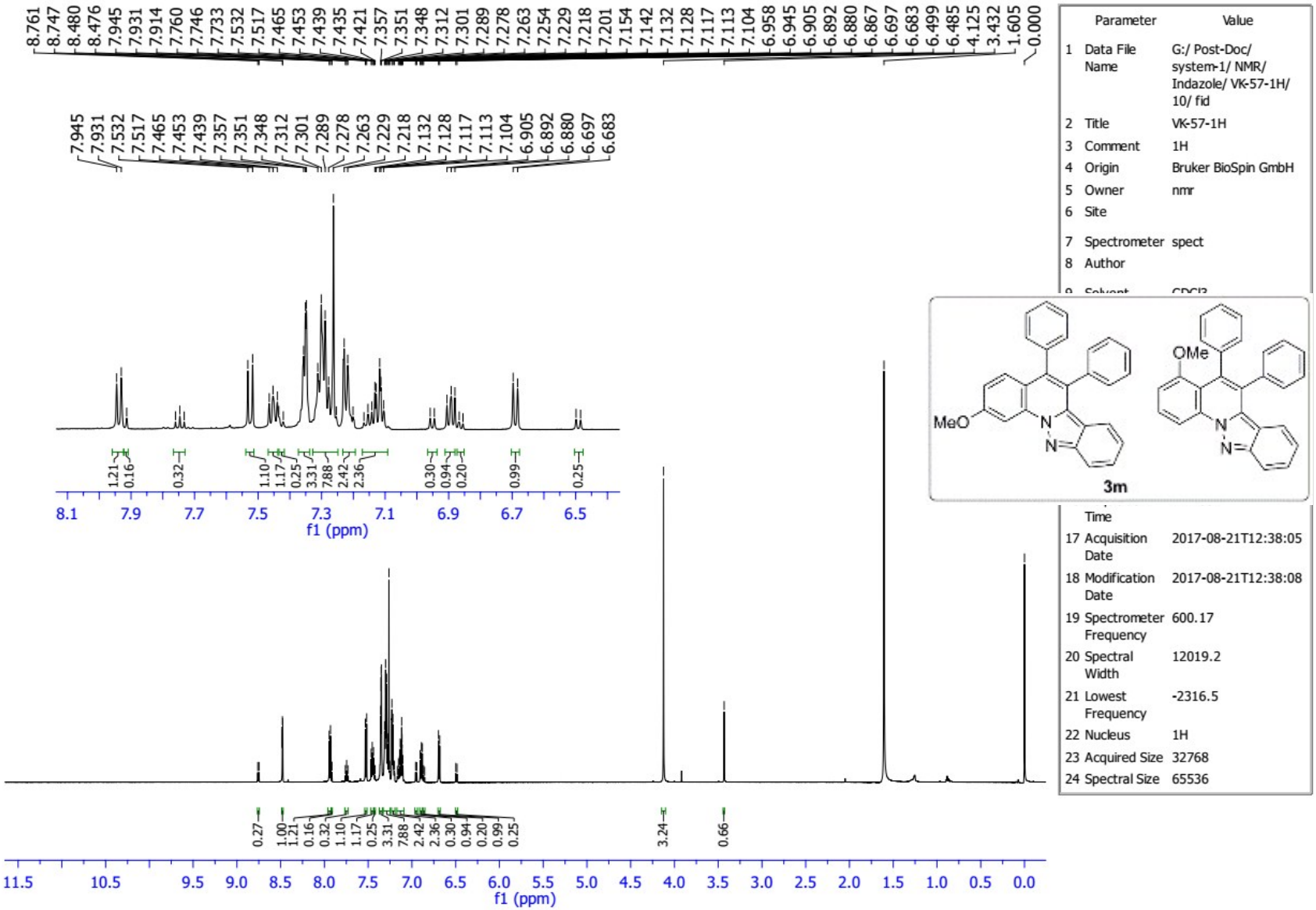
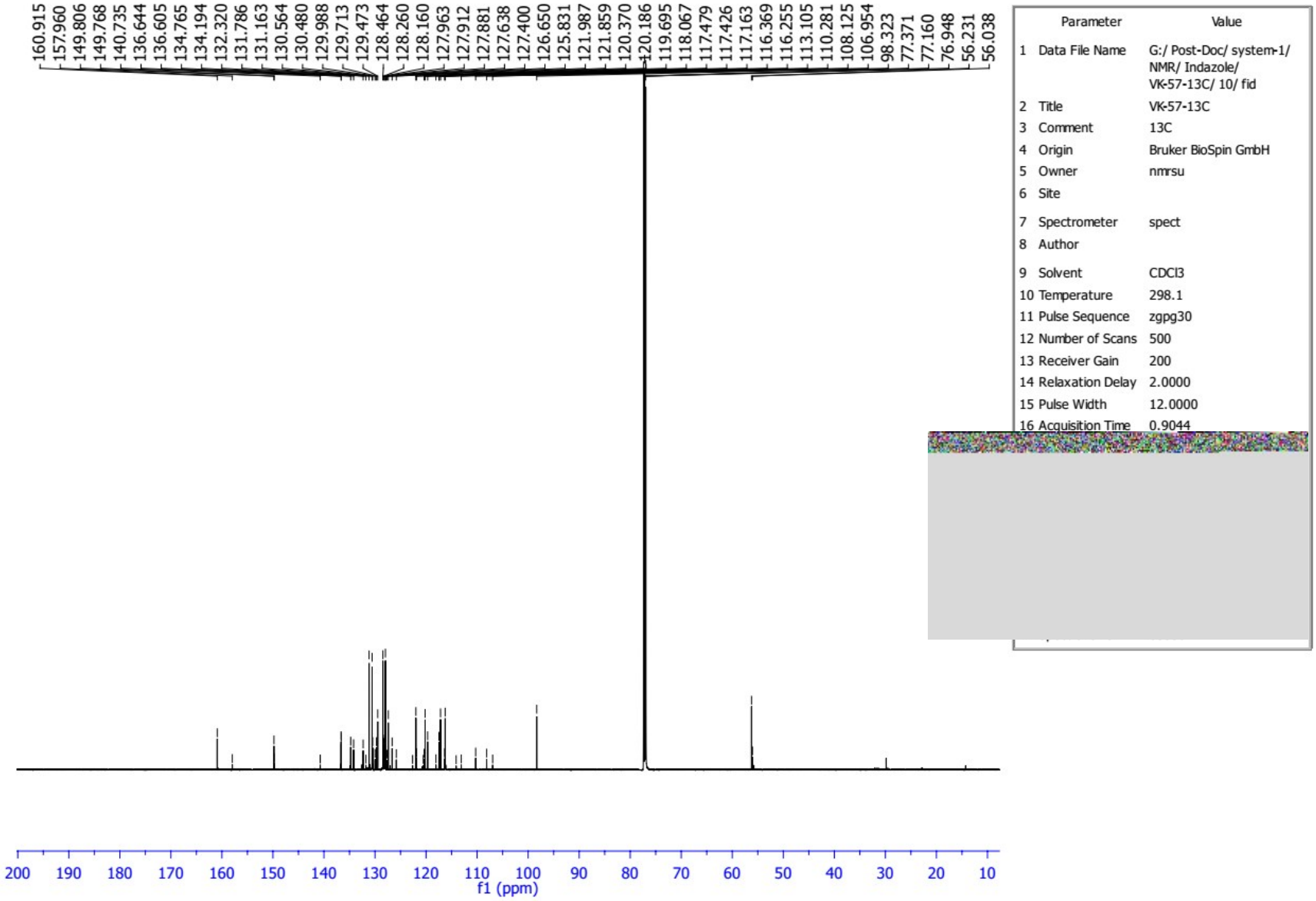
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ 8-9-17-tp/ VK-55-13C/ 10/ fid
2	Title	VK-55-13C
3	Comment	VK-55-13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse	zgpg30
12		
13		
14		
15		
16		
17		
18		
19	Spectrometer Frequency	150.93
20	Spectral Width	36231.9
21	Lowest Frequency	-3003.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	G:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-57-1H/ 10/ fid
2	Title	VK-57-1H
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
	Time	
17	Acquisition Date	2017-08-21T12:38:05
18	Modification Date	2017-08-21T12:38:08
19	Spectrometer Frequency	600.17
20	Spectral Width	12019.2
21	Lowest Frequency	-2316.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536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136.605
134.765
134.194
132.320
131.786
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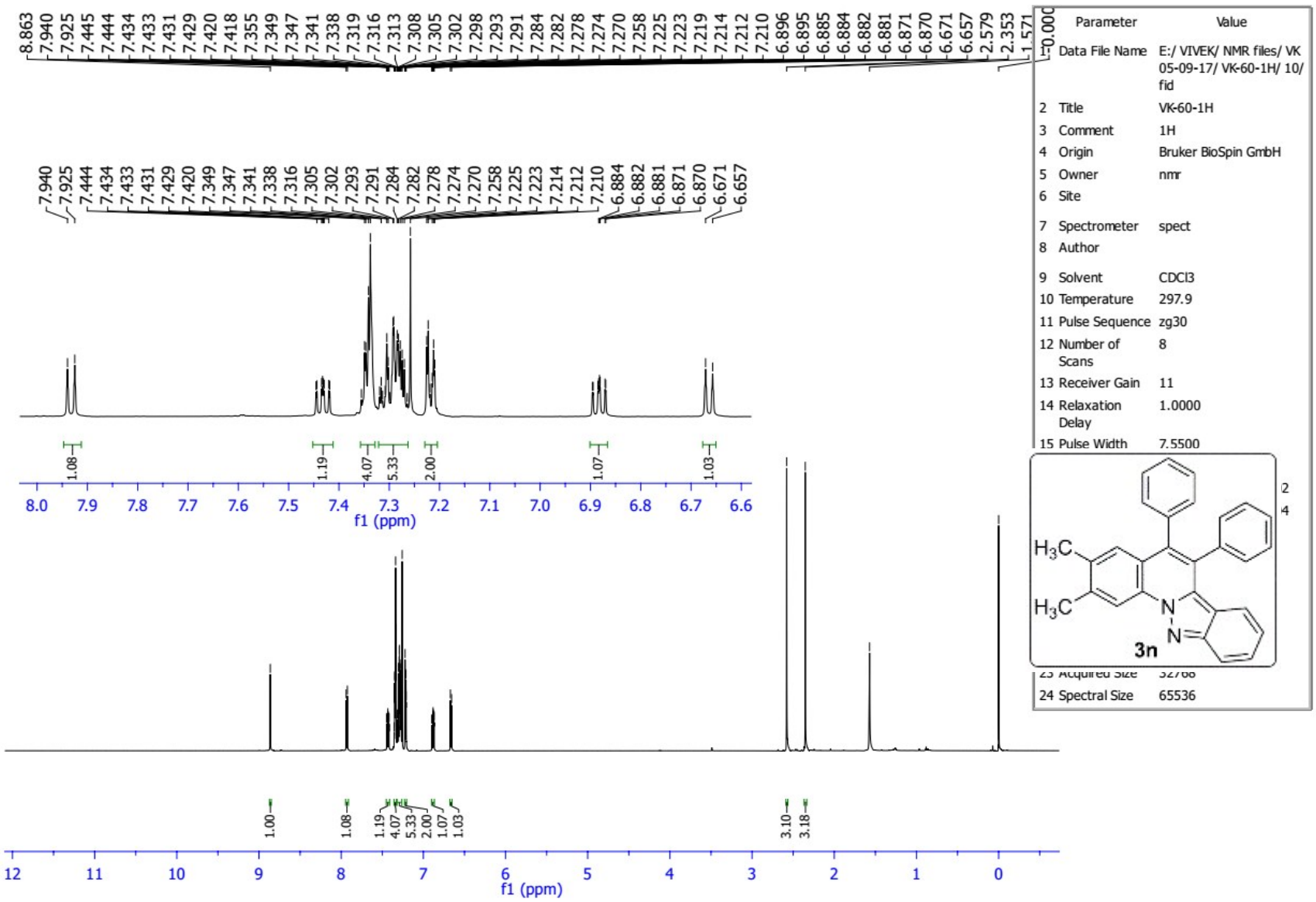
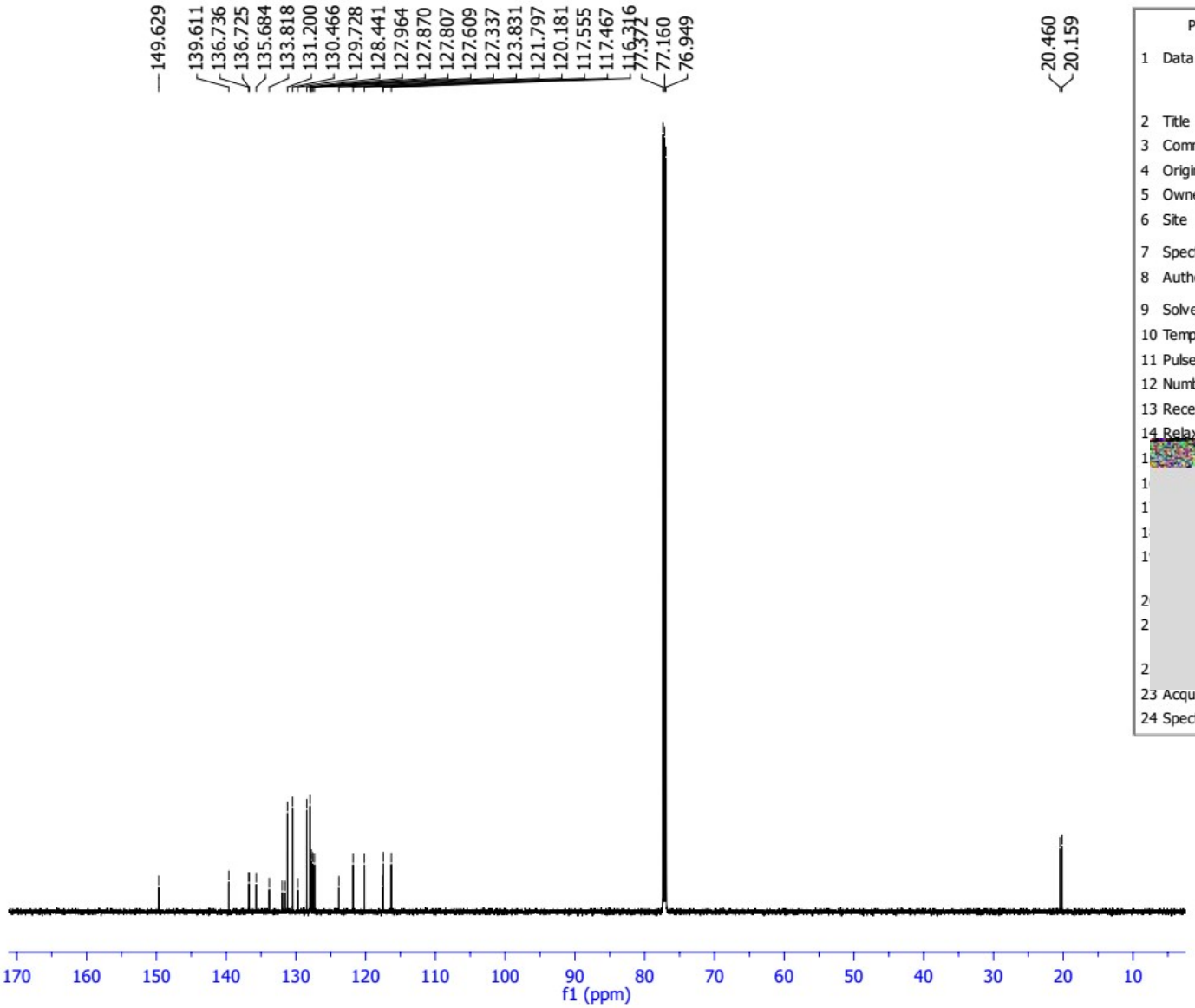
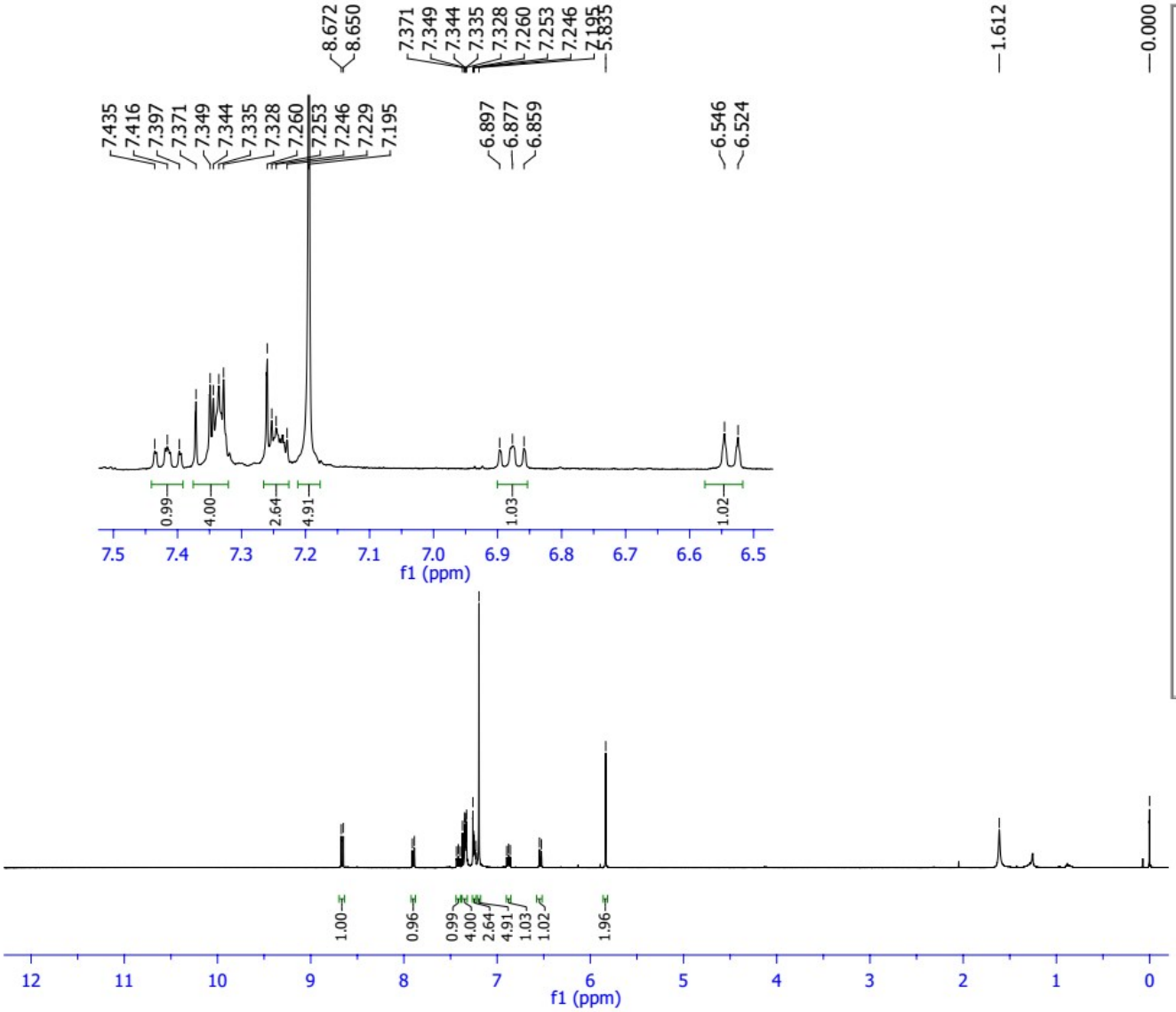
130.564
130.480
129.988
129.713
129.473
128.464
128.260
128.160
127.963
127.912
127.881
127.638
127.400
126.650
125.831
121.987
121.859
120.370
120.186
119.695
118.067
117.479
117.426
117.163
116.369
116.255
113.105
110.281
108.125
106.954
98.323
77.371
77.160
76.948
56.231
56.038
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)
Parameter Value
1 Data File Name G:/ Post-Doc/ system-1/ NMR/ Indazole/ VK-57-13C/ 10/ fid
2 Title VK-57-13C
3 Comment 13C
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zgpg30
12 Number of Scans 500
13 Receiver Gain 200
14 Relaxation Delay 2.0000
15 Pulse Width 12.0000
16 Acquisition Time 0.9044

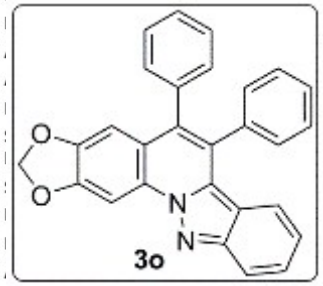

8.863 7.940 7.925 7.445 7.444 7.434 7.433 7.431 7.429 7.420 7.418 7.355 7.349 7.347 7.341 7.338 7.319 7.316 7.313 7.308 7.305 7.302 7.298 7.293 7.291 7.284 7.282 7.278 7.274 7.270 7.258 7.225 7.223 7.219 7.214 7.212 7.210 6.896 6.895 6.885 6.884 6.882 6.881 6.871 6.870 6.671 6.657 2.579 2.353 1.571 0.000
7.940 7.925 7.444 7.434 7.433 7.431 7.429 7.420 7.349 7.347 7.341 7.338 7.316 7.305 7.302 7.293 7.291 7.284 7.282 7.278 7.274 7.270 7.258 7.225 7.223 7.214 7.212 7.210 6.884 6.882 6.881 6.871 6.870 6.671 6.657
1.08 1.19 4.07 5.33 2.00 1.07 1.03
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
f1 (ppm)
1.00 1.08 1.19 4.07 5.33 2.00 1.07 1.03 3.10 3.18
12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
Parameter Value
1 Data File Name E:/ VIVEK/ NMR files/ VK 05-09-17/ VK-60-1H/ 10/ fid
2 Title VK-60-1H
3 Comment 1H
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 297.9
11 Pulse Sequence zg30
12 Number of Scans 8
13 Receiver Gain 11
14 Relaxation Delay 1.0000
15 Pulse Width 7.5500
24 Spectral Size 65536
H3C
H3C
N
N
3n

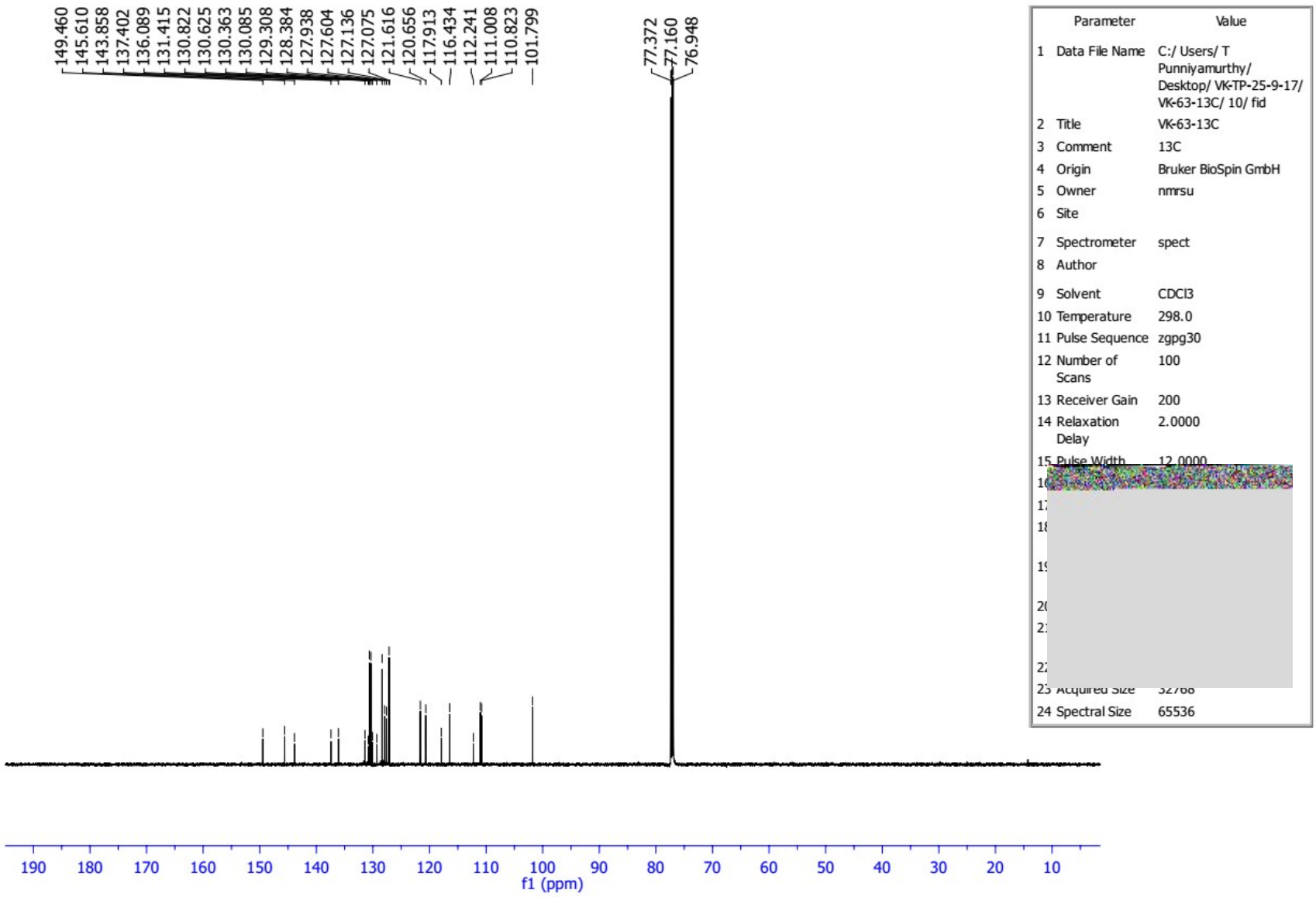


	Parameter	Value
1	Data File Name	E:/ VIVEK/ NMR files/ VK 05-09-17/ VK-60-13C/ 11/ fid
2	Title	VK-60-13C
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Number of Scans	50
13	Receiver Gain	200
14	Relaxation Delay	2.0000
23	Acquired Size	32768
24	Spectral Size	65536

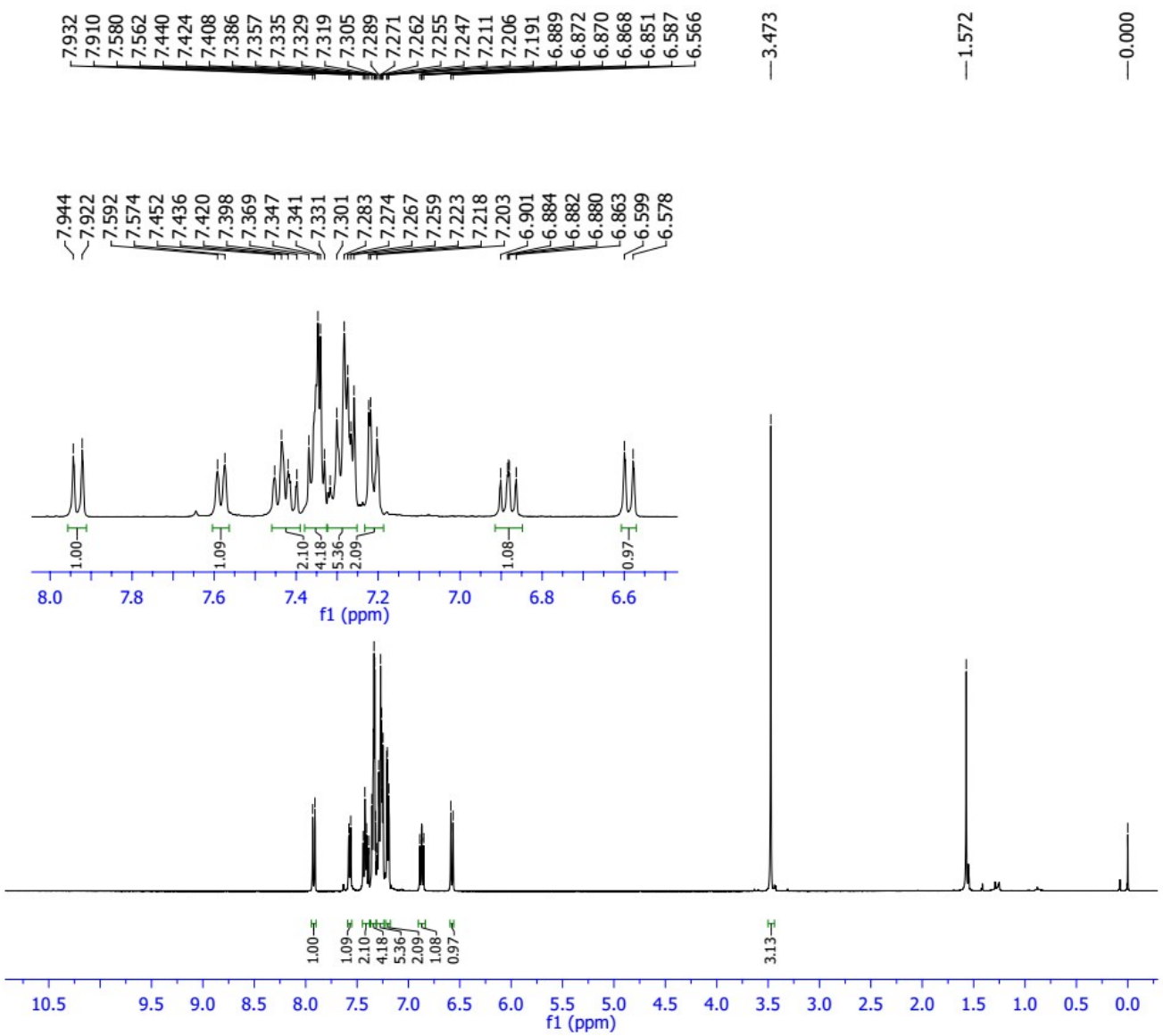


	Parameter	Value
1	Data File Name	H:/ VK-63-1H.fid/ fid
2	Title	VK-63-1H
3	Comment	VK-63-1H
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	mercury
8	Author	
9	Solvent	cdcl3
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	16
13	Receiver Gain	30
14	Relaxation Delay	1.0000
15		
16		
17		
18		
19		
20		
21		
22		
23		
24	Spectral Size	32768

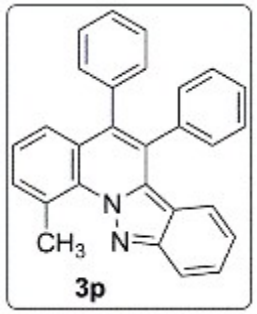




	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-TP-25-9-17/ VK-63-13C/ 10/ fid
2	Title	VK-63-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	100
13	Receiver Gain	200
14	Relaxation Delay	2.0000
15	Pulse Width	12.0000
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ VK-65-1H.fid/ fid
2	Title	VK-65-1H
3	Comment	VK-65-1H
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	mercury
8	Author	
9	Solvent	cdcl3
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	32
13	Receiver Gain	30
24	Spectral Size	32768



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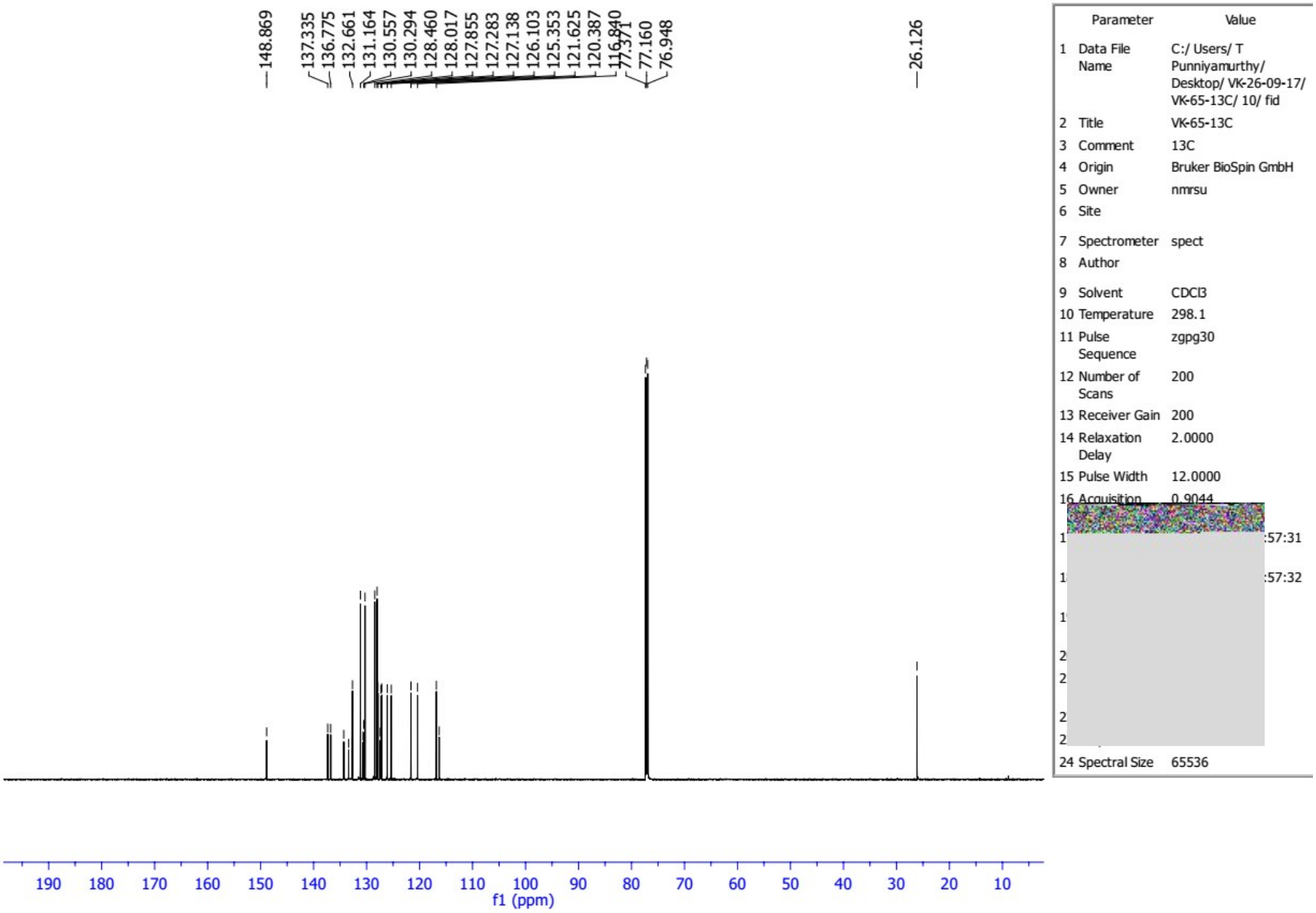
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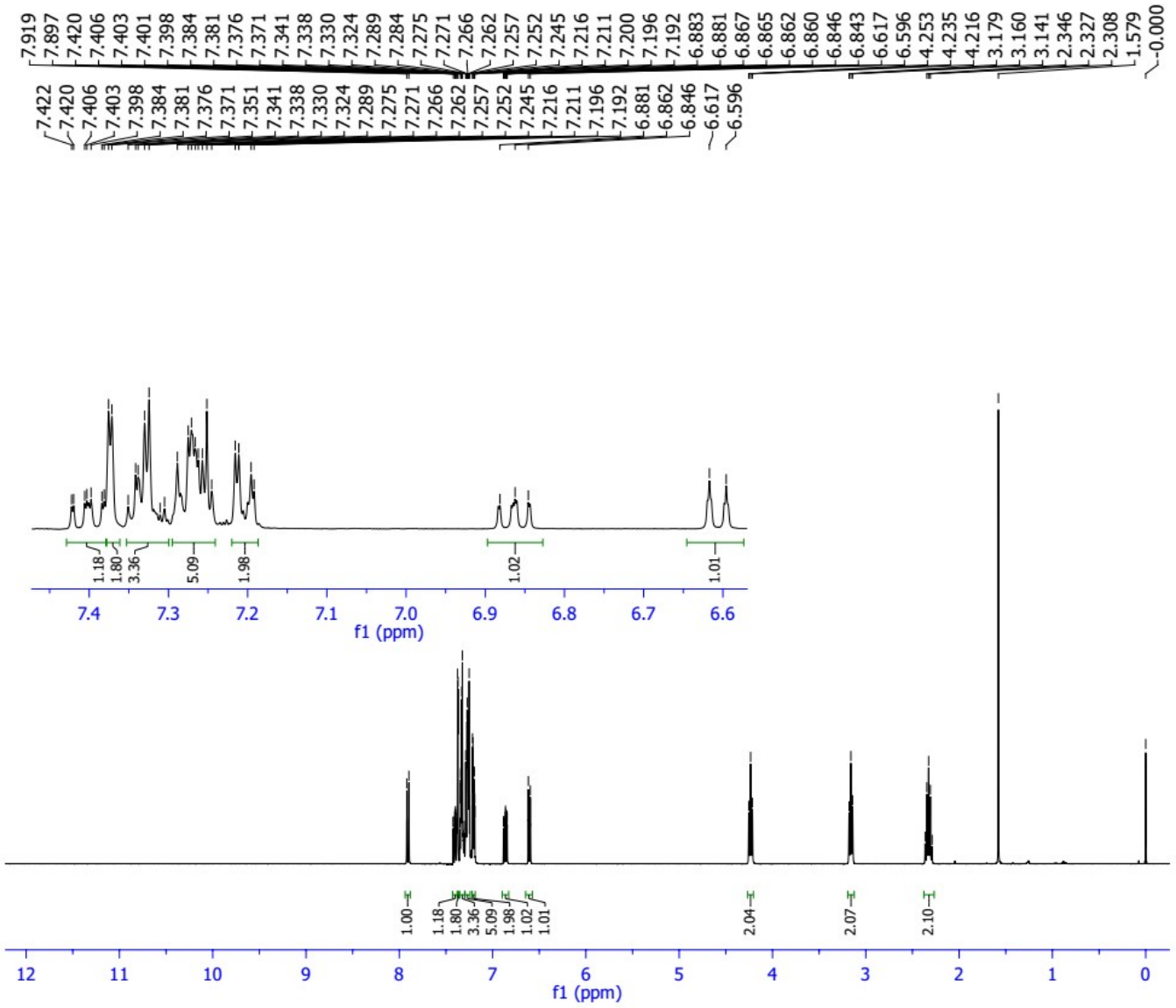
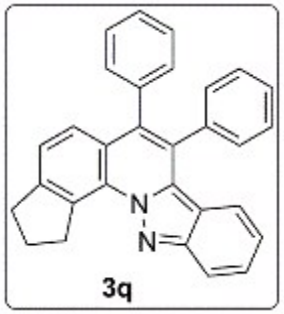
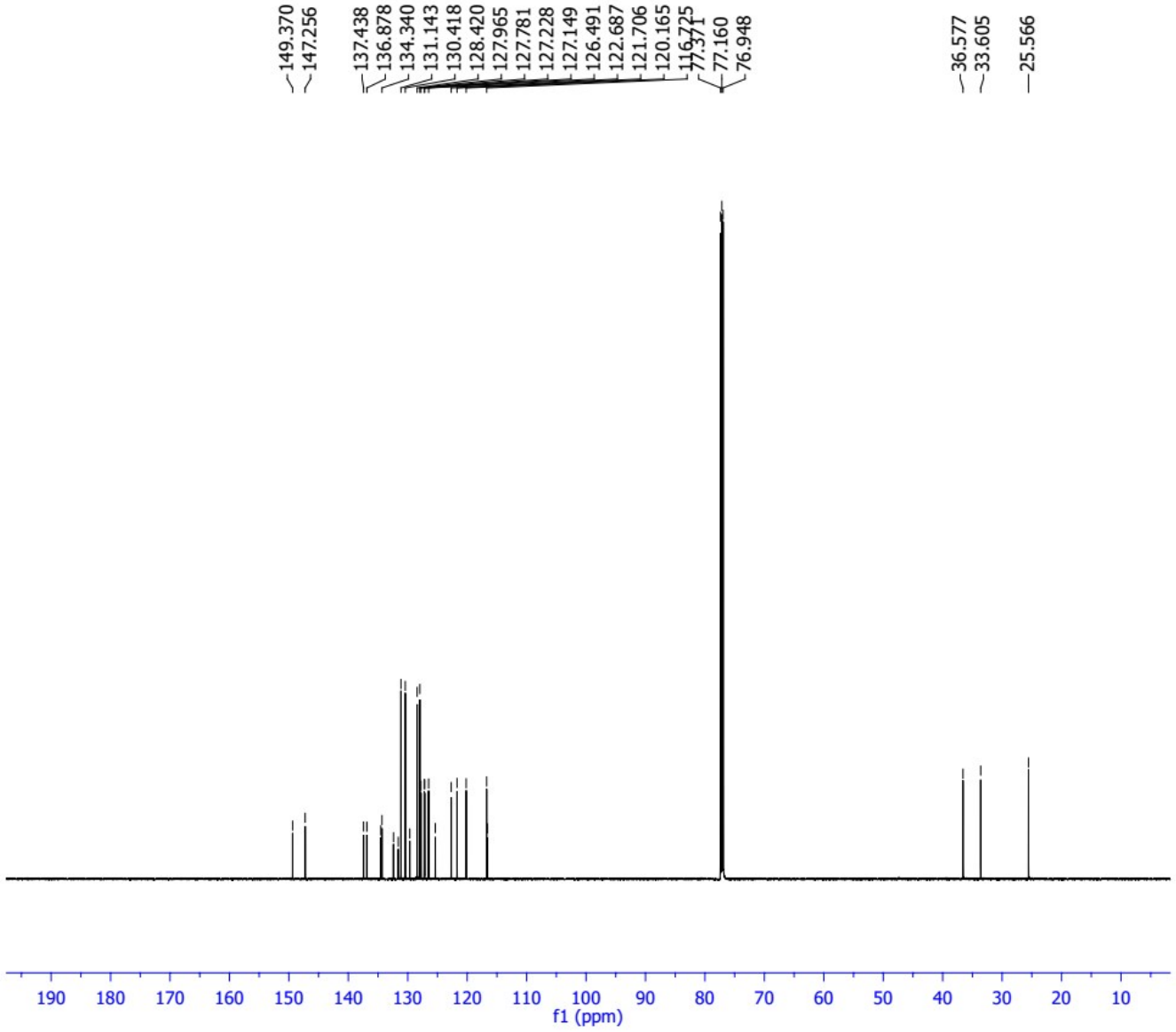
132.661
131.164
130.557
130.294
128.460
128.017
127.855
127.283
127.138
126.103
125.353
121.625
120.387
116.840
77.371
77.160
76.948
26.126
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ T Punniyamurthy/ Desktop/ VK-26-09-17/ VK-65-13C/ 10/ fid
2 Title VK-65-13C
3 Comment 13C
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zgpg30
12 Number of Scans 200
13 Receiver Gain 200
14 Relaxation Delay 2.0000
15 Pulse Width 12.0000
16 Acquisition 0.9044
:57:31
:57:32
24 Spectral Size 65536

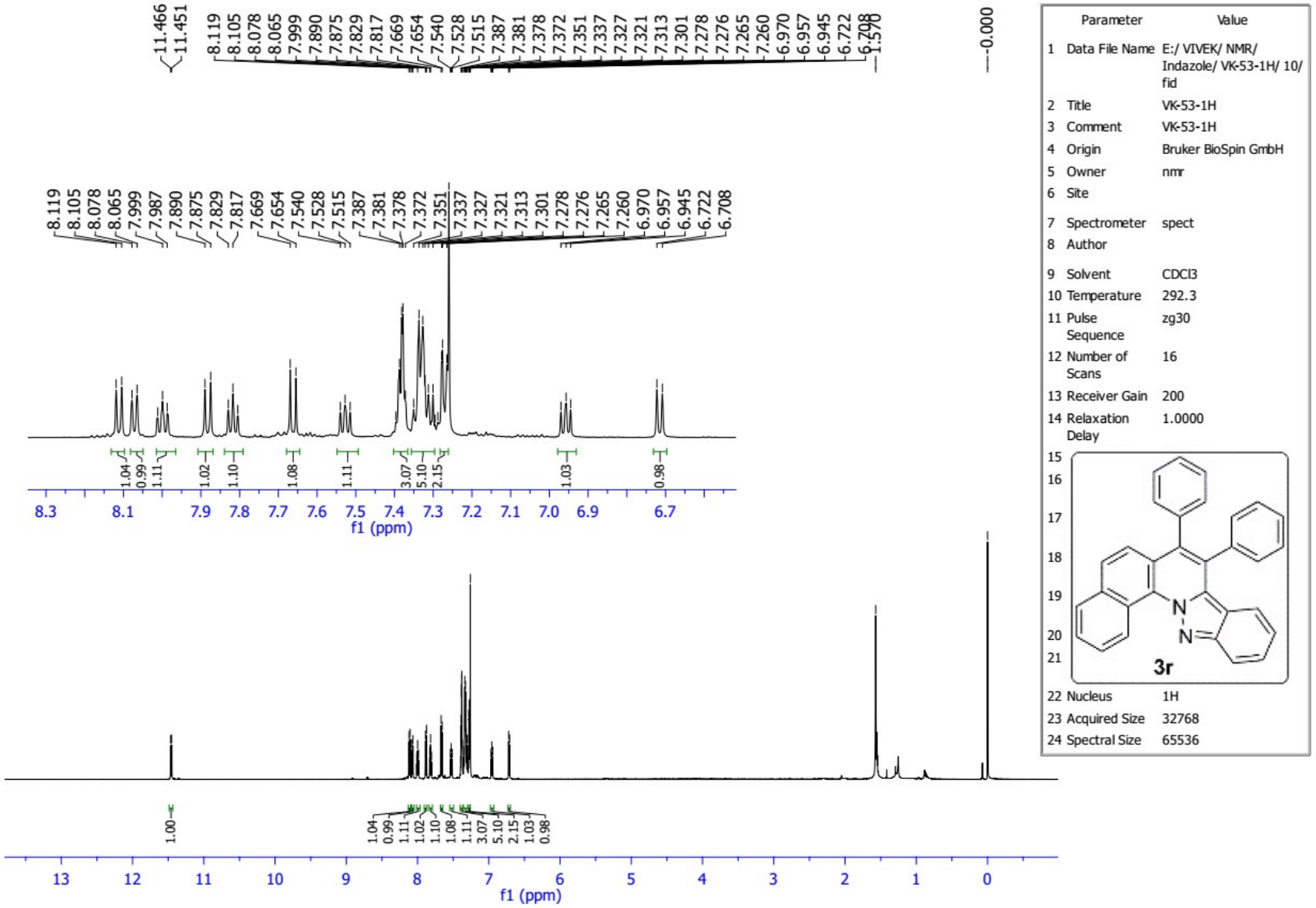


	Parameter	Value
1	Data File Name	E:/ VK-64-1H.fid/ fid
2	Title	VK-64-1H
3	Comment	VK-64-1H
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	mercury
8	Author	
9	Solvent	cdcl3
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	28
13	Receiver Gain	30
14	Relaxation Delay	1.0000
15		
16		
17		
18		
19		
20		
21		
	Frequency	
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

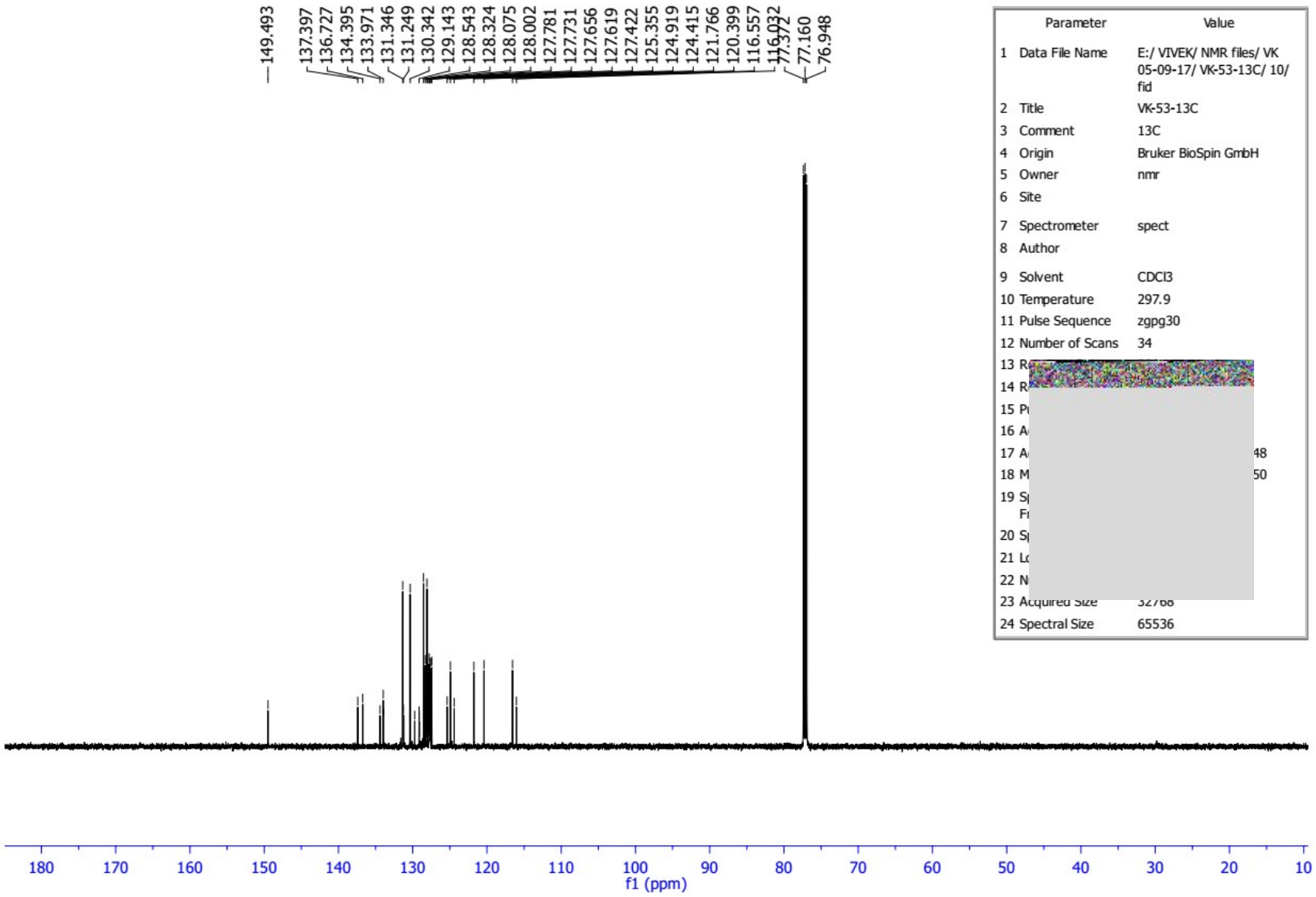




	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-26-09-17/ VK-64-13C/ 10/ fid
2	Title	VK-64-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Number of Scans	200
13	Receiver Gain	200
14		
15		
16		
17		
18		
19		
20	Width	
21	Lowest Frequency	-3005.8
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ VIVEK/ NMR/ Indazole/ VK-53-1H/ 10/ fid
2	Title	VK-53-1H
3	Comment	VK-53-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	200
14	Relaxation Delay	1.0000
15		
16		
17		
18		
19		
20		
21		
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536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131.249
130.342
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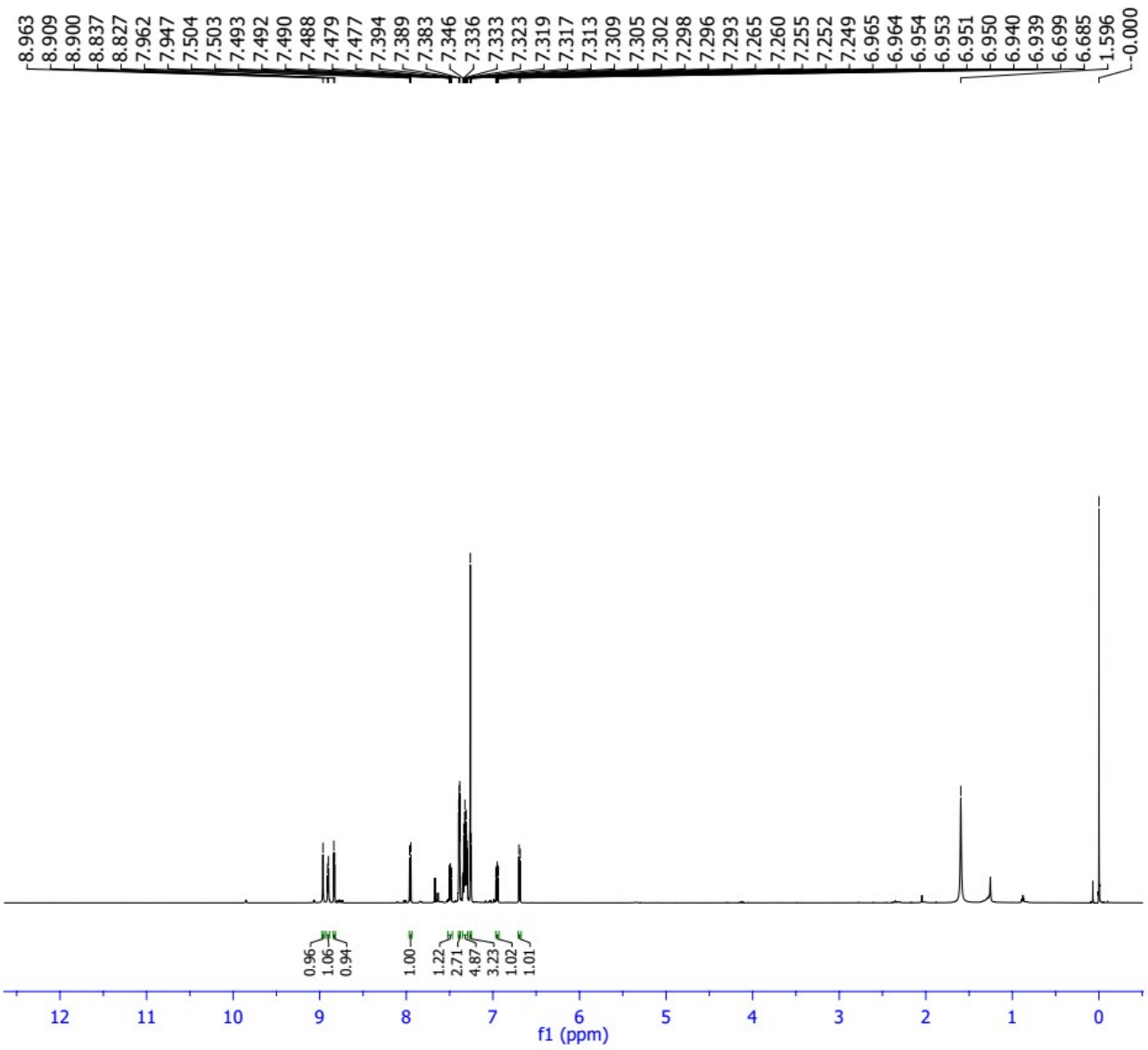
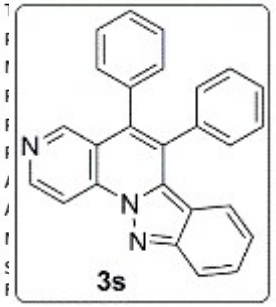
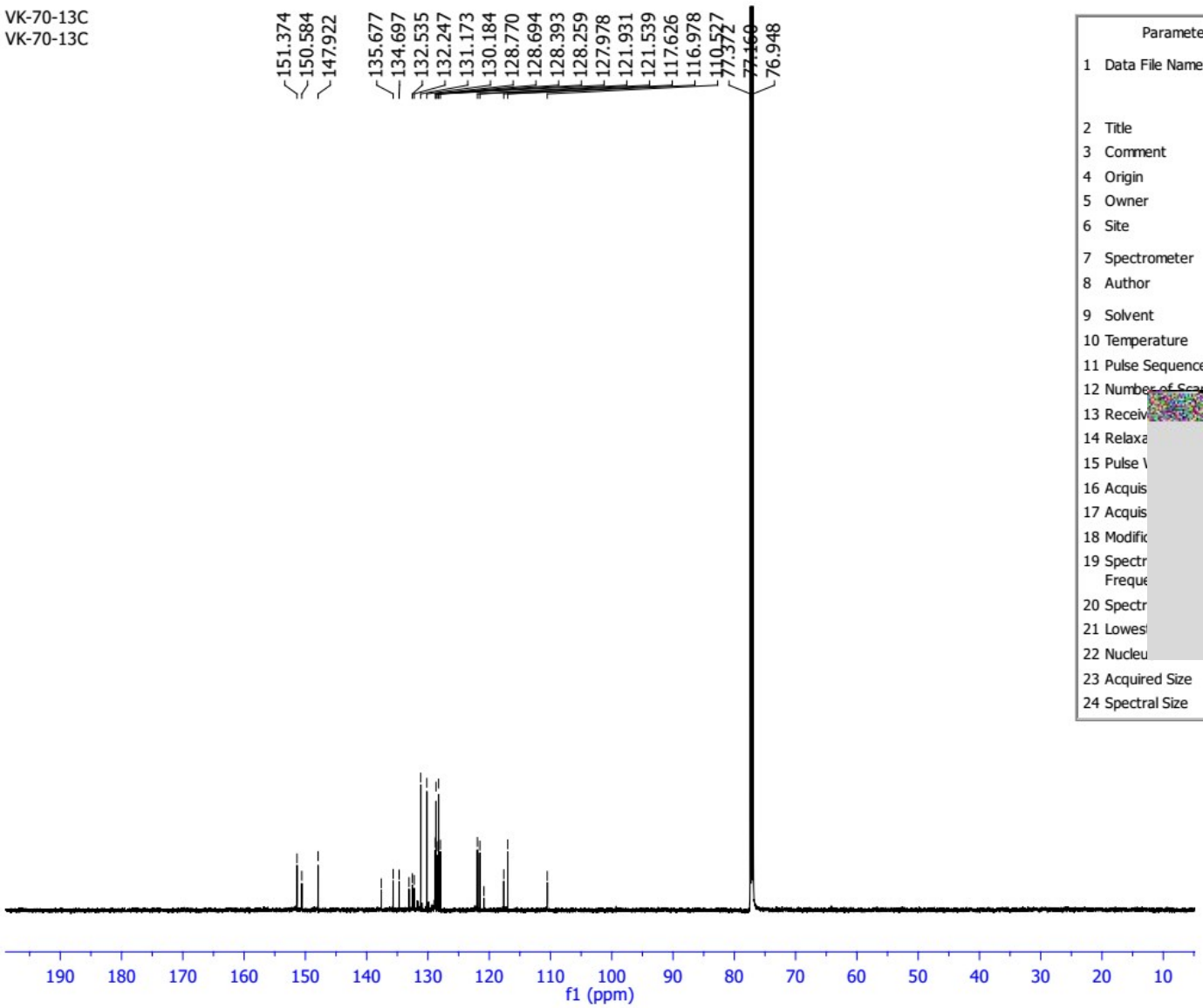
128.543
128.324
128.075
128.002
127.781
127.731
127.656
127.619
127.422
125.355
124.919
124.415
121.766
120.399
116.557
116.032
77.372
77.160
76.948
Parameter
Value
1 Data File Name
E:/ VIVEK/ NMR files/ VK 05-09-17/ VK-53-13C/ 10/ fid
2 Title
VK-53-13C
3 Comment
13C
4 Origin
Bruker BioSpin GmbH
5 Owner
nmr
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
297.9
11 Pulse Sequence
zgpg30
12 Number of Scans
34
23 Acquired Size
32768
24 Spectral Size
65536
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

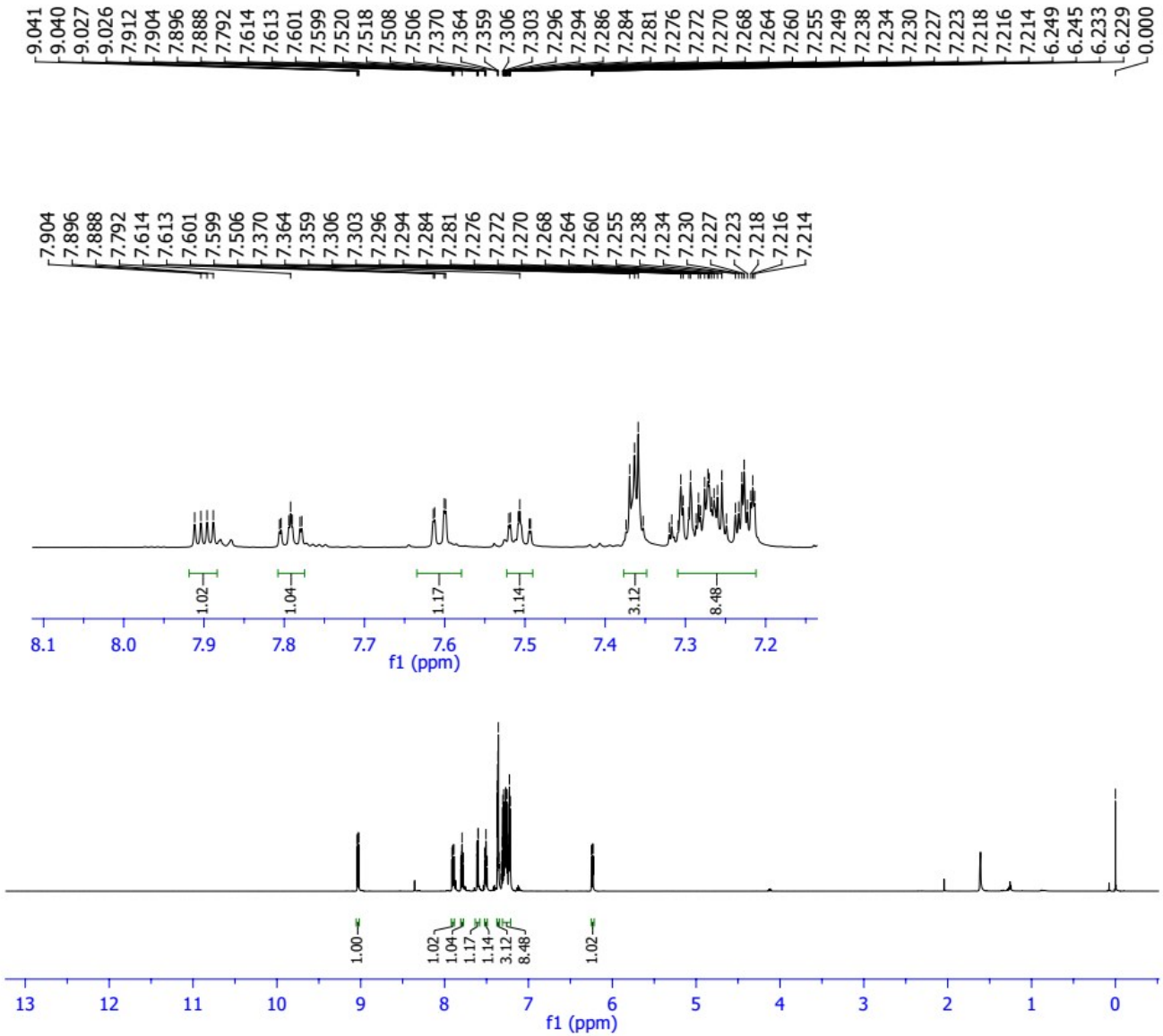


	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-4-12-2017/ VK-70-1H/ 10/ fid
2	Title	VK-70-1H
3	Comment	VK-70-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10		
11		
12		
13		
14		
15		
16		
17		00:40
18		00:42
19		
20	Spectral Width	12019.2
21	Lowest Frequency	-2317.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

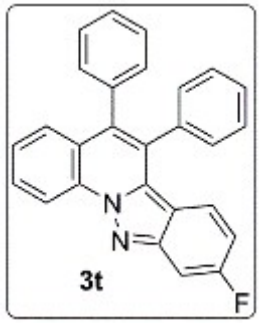


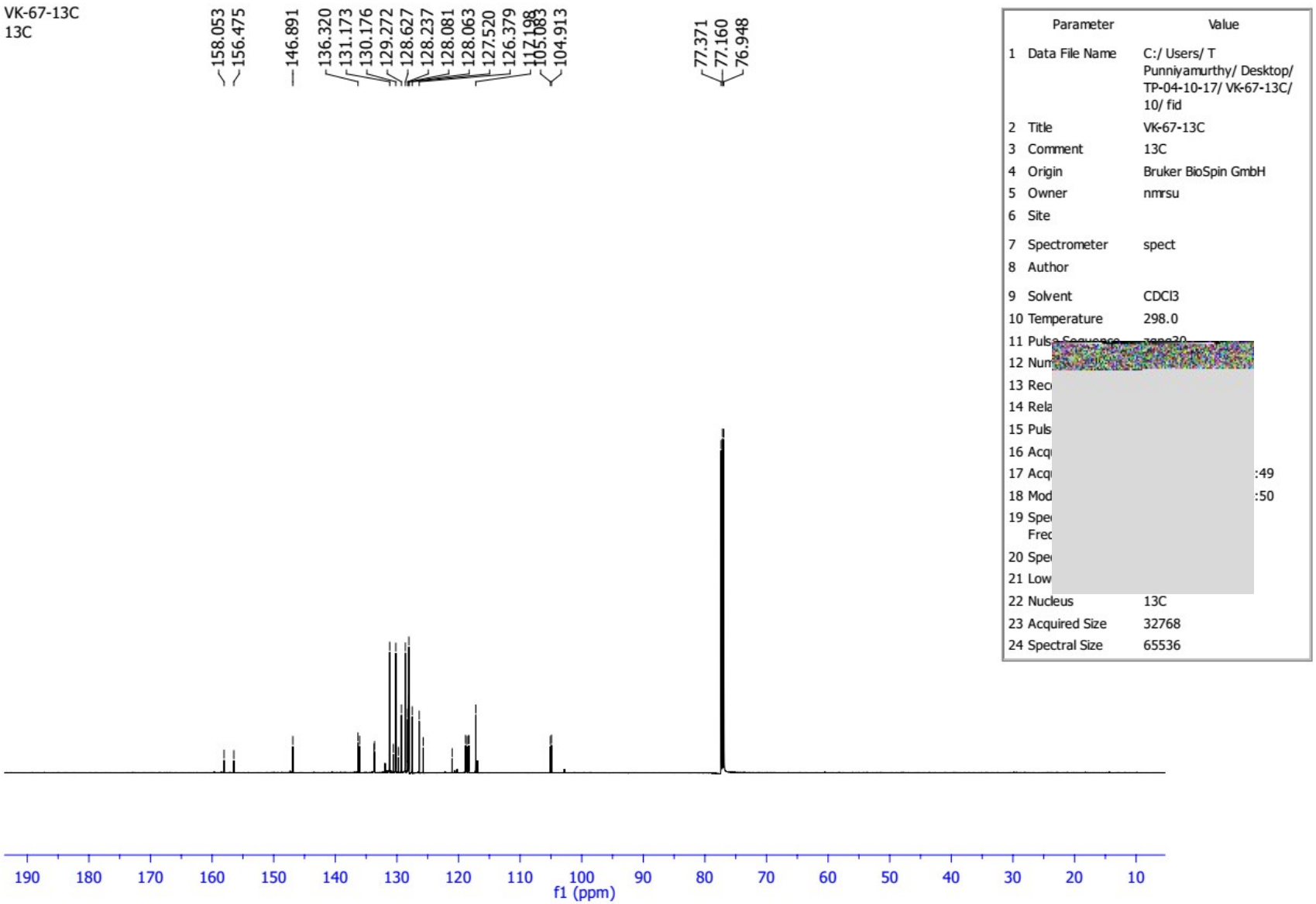


	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-4-12-2017/ VK-70-13C/ 10/ fid
2	Title	VK-70-13C
3	Comment	VK-70-13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	500
13	Receiv	
14	Relaxa	
15	Pulse V	
16	Acquis	
17	Acquis	31
18	Modific	32
19	Spectr Freque	
20	Spectr	
21	Lowest	
22	Nucleu	
23	Acquired Size	32768
24	Spectral Size	65536



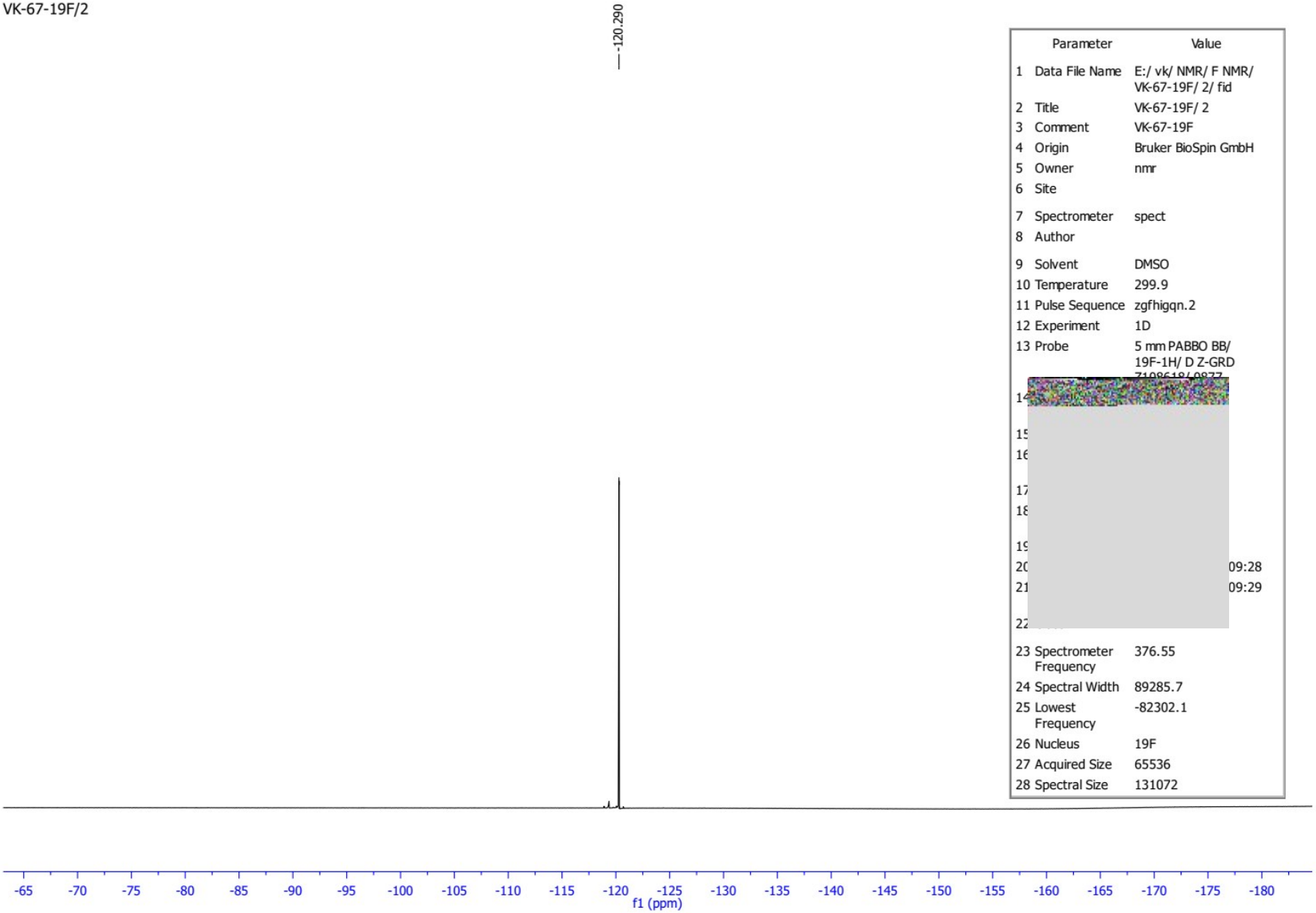
	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ TP-04-10-17/ VK-67-1H/ 10/ fid
2	Title	VK-67-1H
3	Comment	1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	10
14	Relaxation Delay	1.0000
15	Pu	
16	Ac	
17	Ac	
18	Mc	
19	Sp Fr	
20	Sp	
21	Lo Fr	
22	Nu	
23	Ac	
24	Sp	



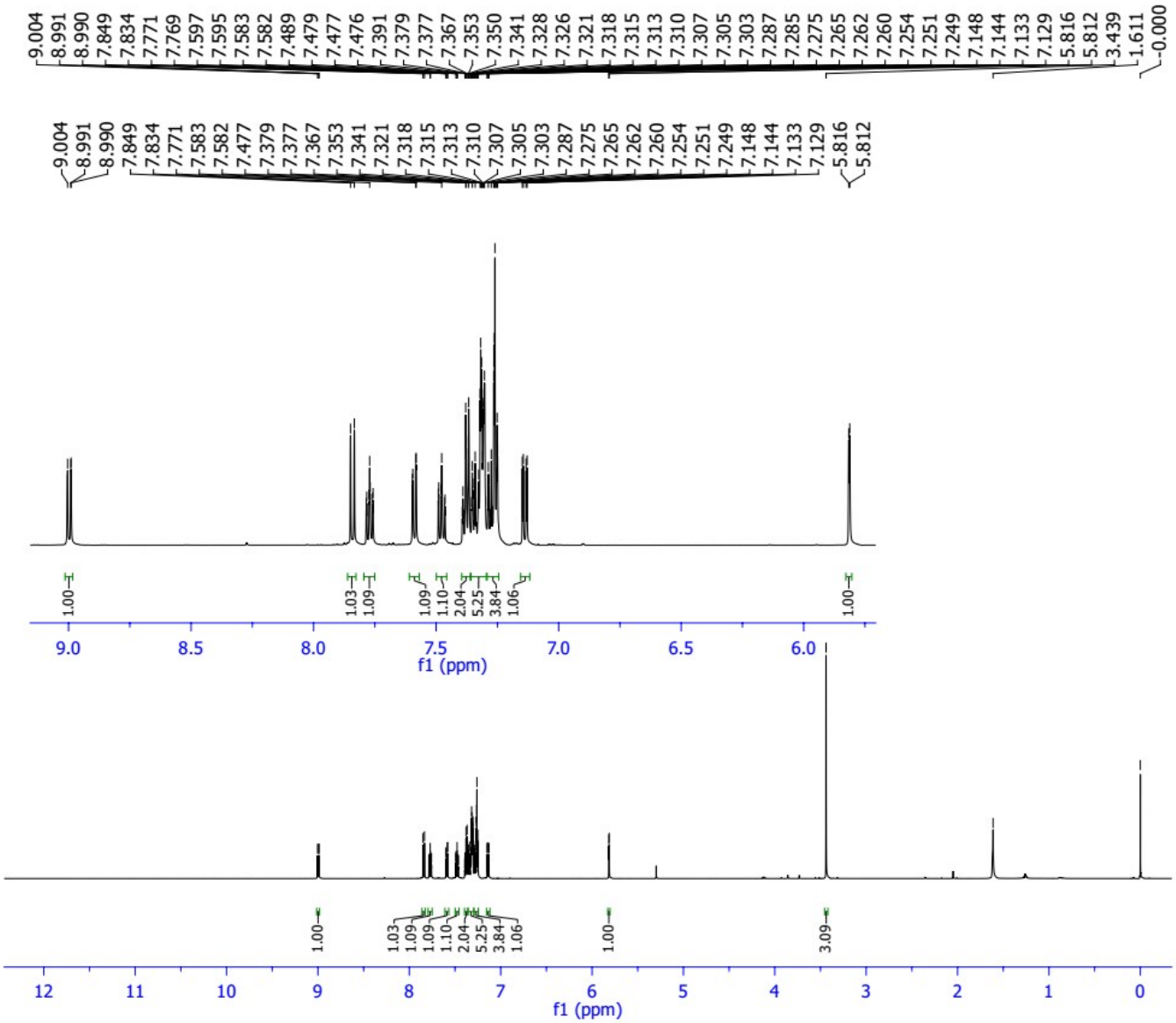


	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ TP-04-10-17/ VK-67-13C/ 10/ fid
2	Title	VK-67-13C
3	Comment	13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	[illegible]
12	Num[illegible]	
13	Rec[illegible]	
14	Rela[illegible]	
15	Puls[illegible]	
16	Acq[illegible]	
17	Acq[illegible]	:49
18	Mod[illegible]	:50
19	Spe[illegible] Frec[illegible]	
20	Spe[illegible]	
21	Low[illegible]	
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

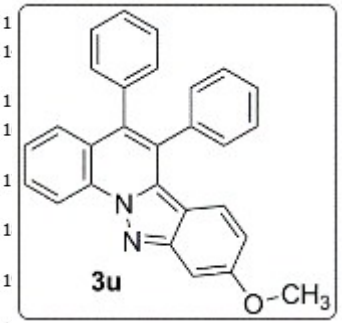
VK-67-19F/2

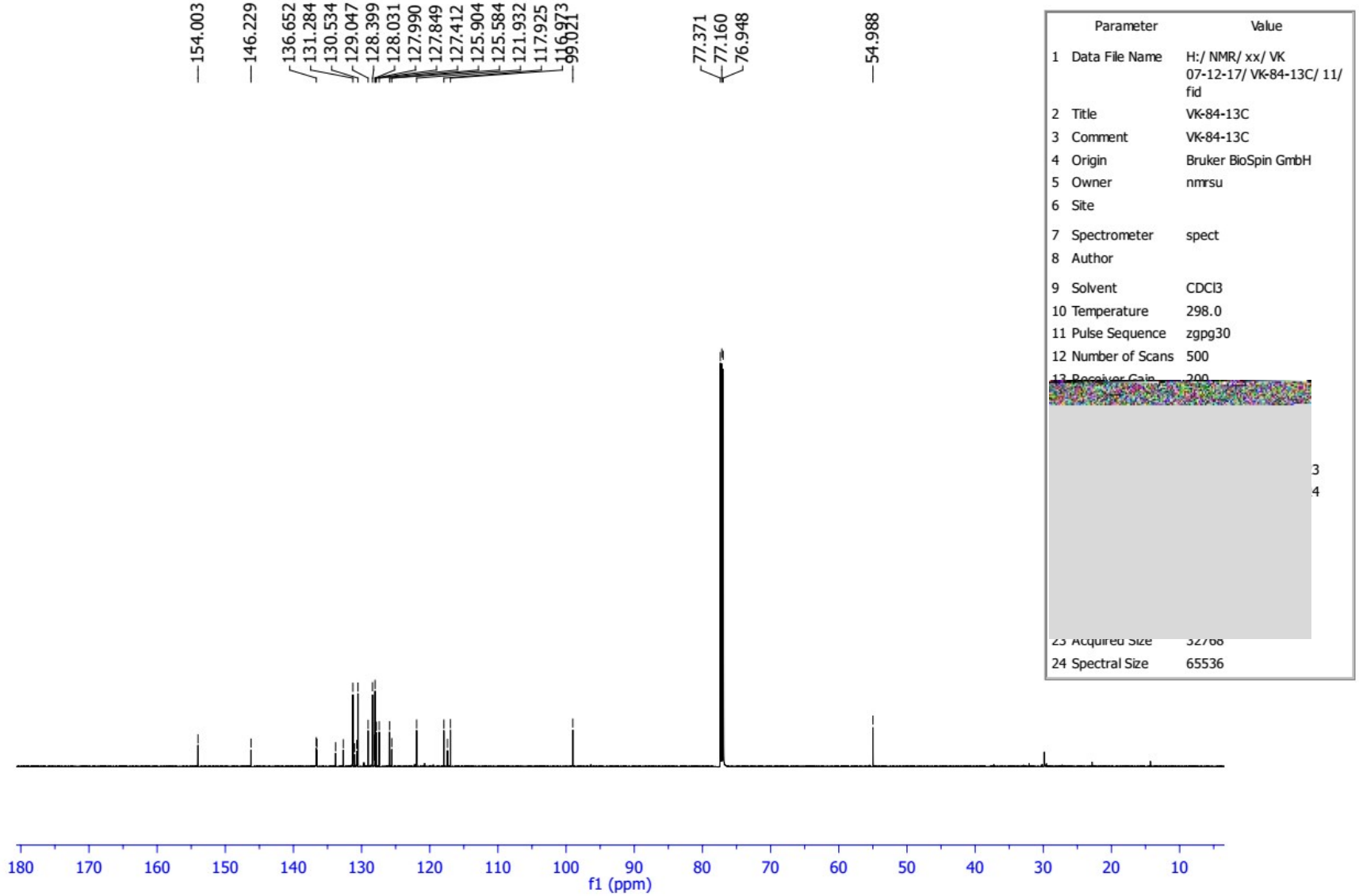


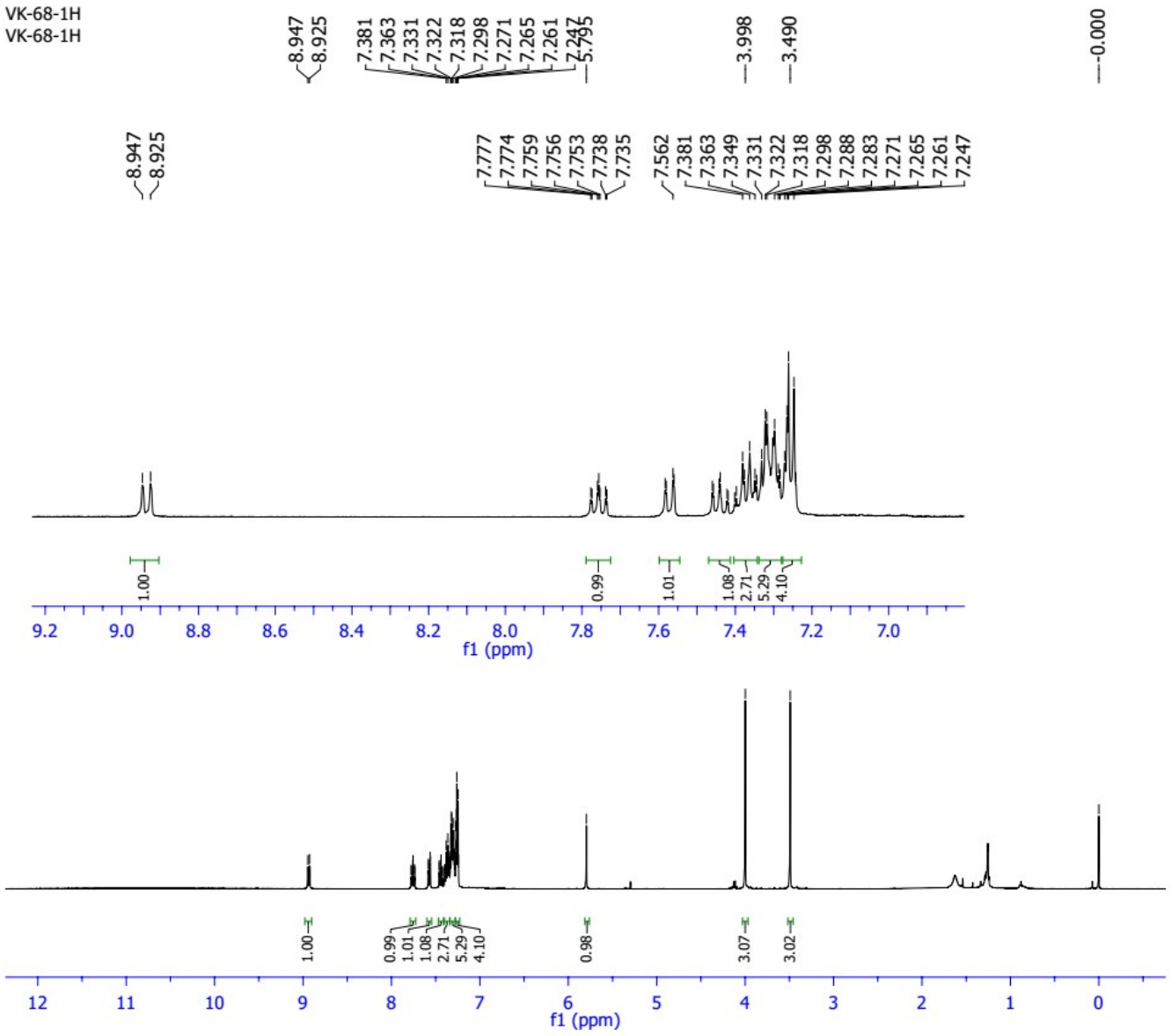
	Parameter	Value
1	Data File Name	E:/ vk/ NMR/ F NMR/ VK-67-19F/ 2/ fid
2	Title	VK-67-19F/ 2
3	Comment	VK-67-19F
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	299.9
11	Pulse Sequence	zgfhigqn.2
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD
14		
15		
16		
17		
18		
19		
20		09:28
21		09:29
22		
23	Spectrometer Frequency	376.55
24	Spectral Width	89285.7
25	Lowest Frequency	-82302.1
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072



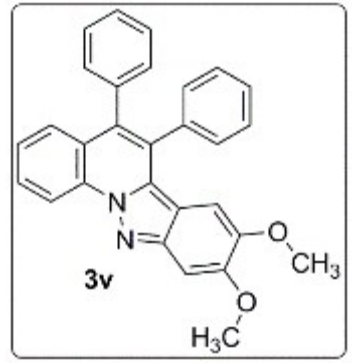
	Parameter	Value
1	Data File Name	H:/ NMR/ xx/ VK-84A-1H/ 10/ fid
2	Title	VK-84A-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	8
20	Spectral Width	12019.2
21	Lowest Frequency	-2316.8
22	Nucleus	1H

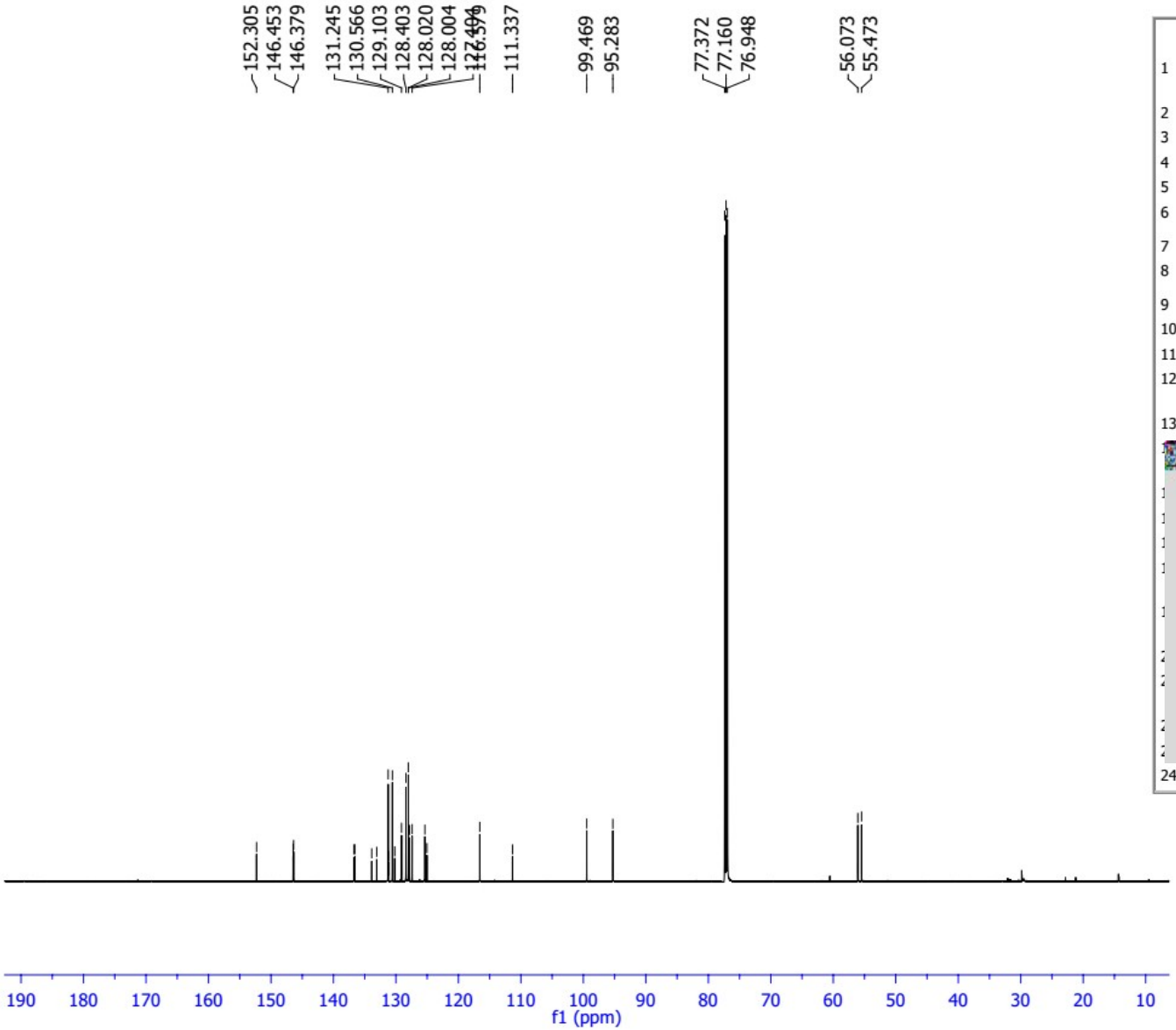



154.003
146.229
136.652
131.284
130.534
129.047
128.399
128.031
127.990
127.849
127.412
125.904
125.584
121.932
117.925
116.973
99.021
77.371
77.160
76.948
54.988
Parameter
Value
1 Data File Name
H:/ NMR/ xx/ VK 07-12-17/ VK-84-13C/ 11/ fid
2 Title
VK-84-13C
3 Comment
VK-84-13C
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
298.0
11 Pulse Sequence
zgpg30
12 Number of Scans
500
24 Spectral Size
65536
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

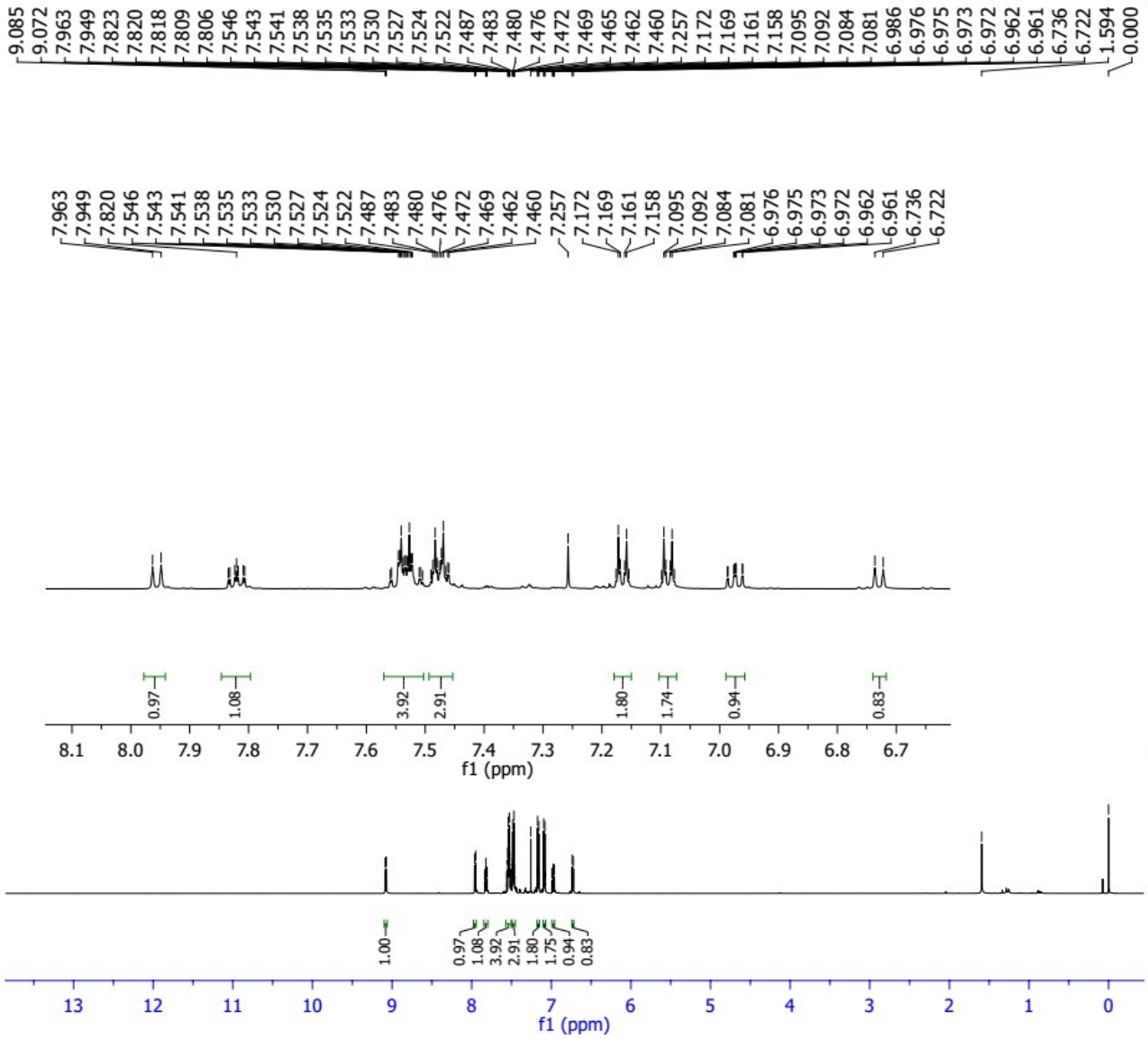


	Parameter	Value
1	Data File Name	E:/ VIVEK/ VK-68-1H.fid/ fid
2	Title	VK-68-1H
3	Comment	VK-68-1H
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	mercury
8	Author	
9	Solvent	cdcl3
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	32
13	Receiver Gain	30
14	Relaxation	1.0000
23	Acquired Size	16384
24	Spectral Size	32768

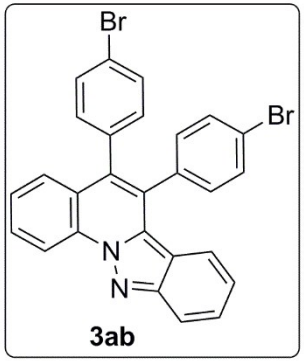


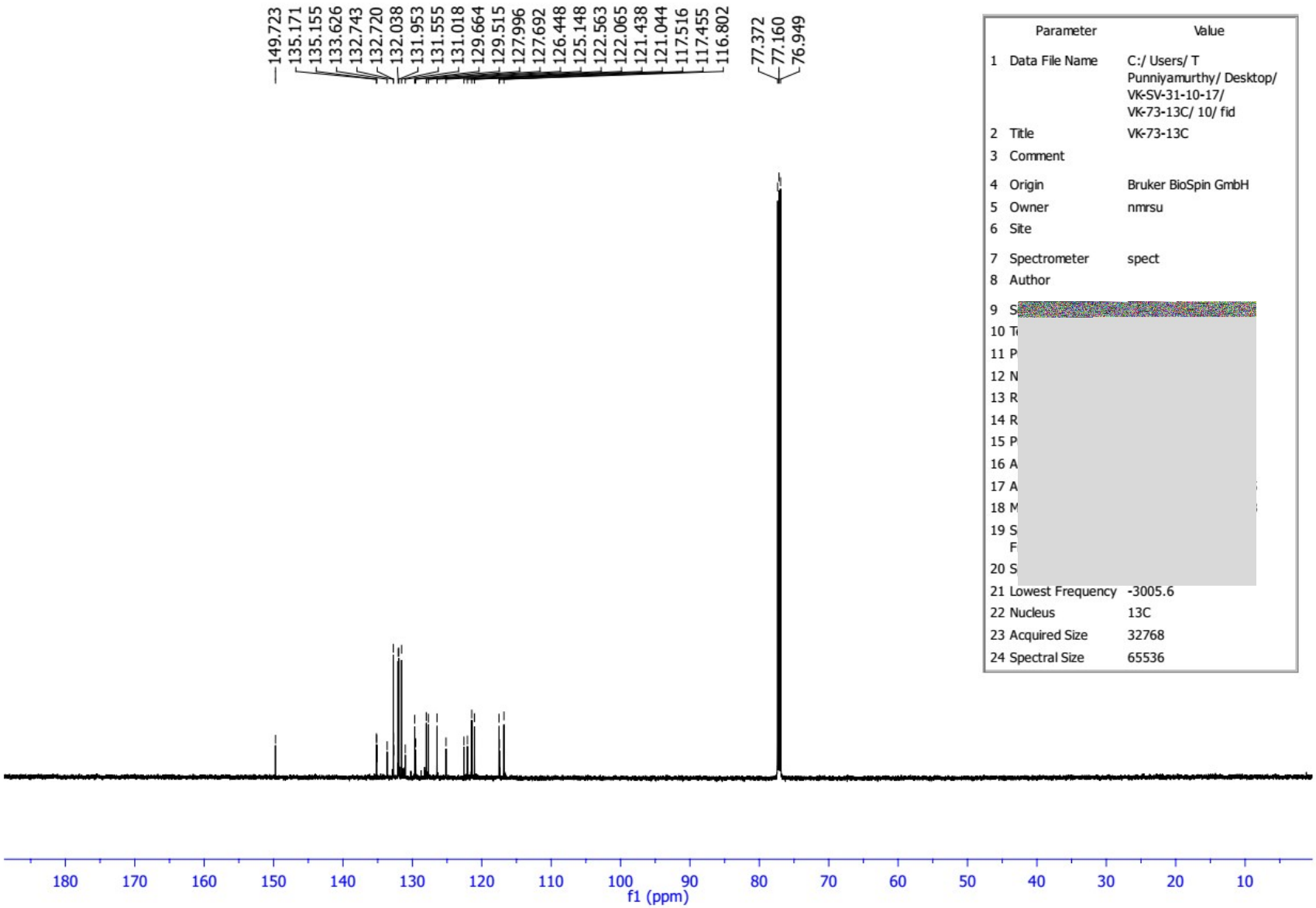


	Parameter	Value
1	Data File Name	H:/ NMR/ xx/ VK-68-13C/ 1/ fid
2	Title	VK-68-13C
3	Comment	VK-68-13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	500
13	Receiver Gain	200
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop// VK-73A-1H/ 10/ fid
2	Title	VK-73A-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12		
13		
14		
15		
16		
17		:58
18		:00
19		
20		
21		
22		
23		
24	Spectral Size	65536




149.723
135.171
135.155
133.626
132.743
132.720
132.038
131.953
131.555
131.018
129.664
129.515
127.996
127.692
126.448
125.148
122.563
122.065
121.438
121.044
117.516
117.455
116.802
77.372
77.160
76.949
Parameter Value
1 Data File Name C:/ Users/ T Punniyamurthy/ Desktop/ VK-SV-31-10-17/ VK-73-13C/ 10/ fid
2 Title VK-73-13C
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
21 Lowest Frequency -3005.6
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536
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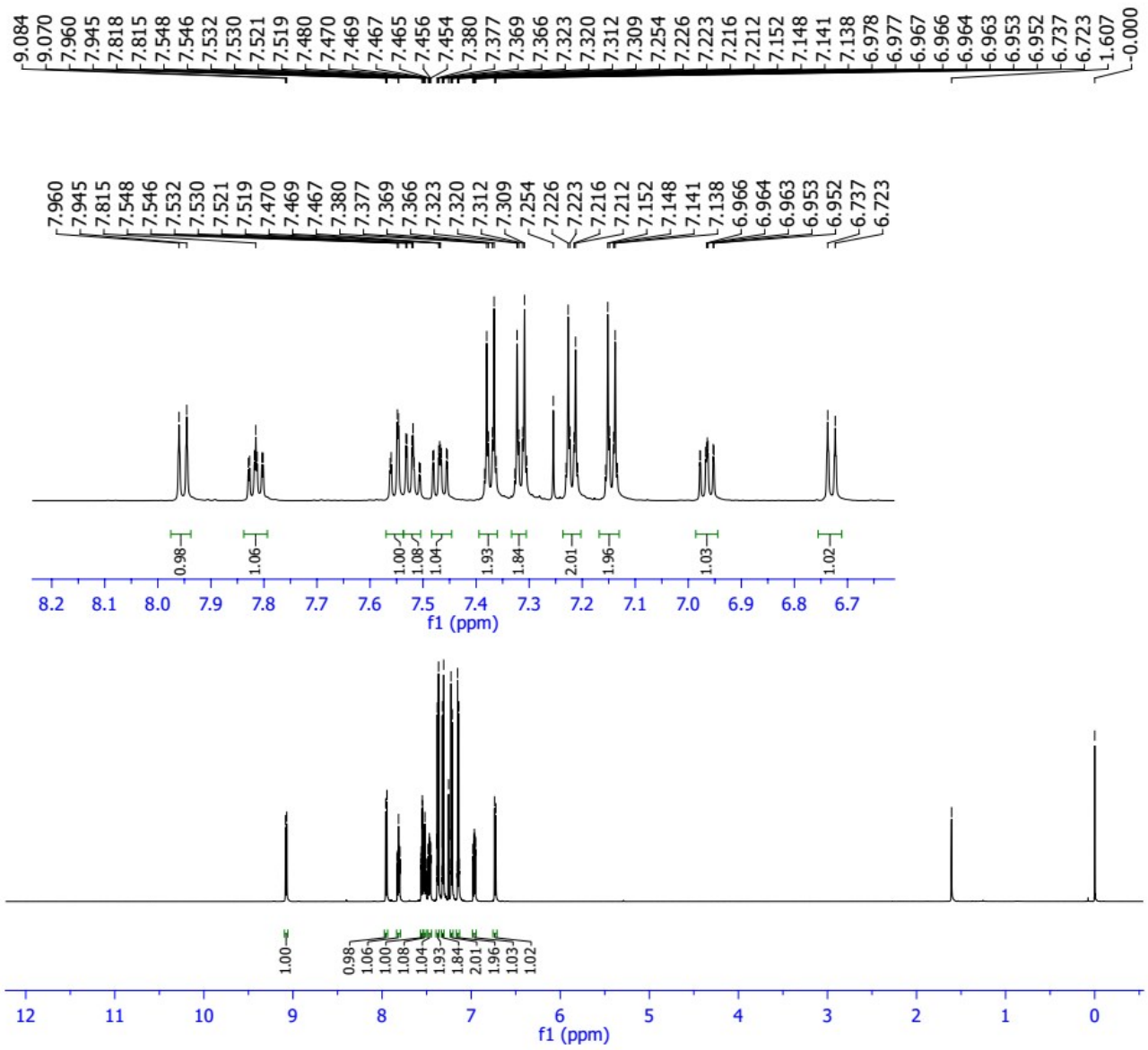
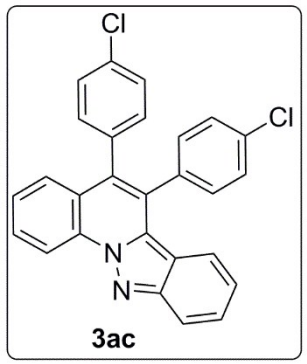
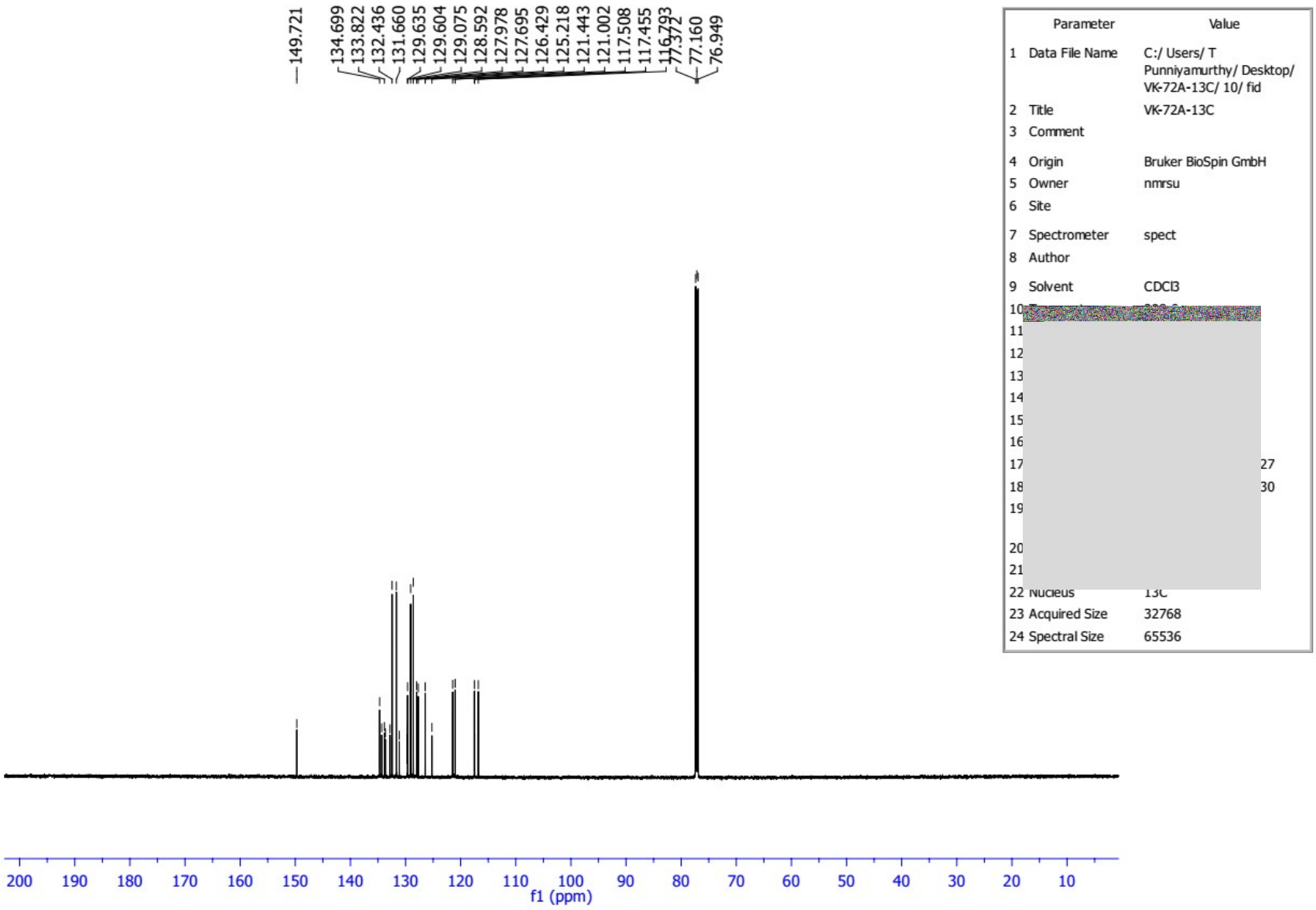
f1 (ppm)

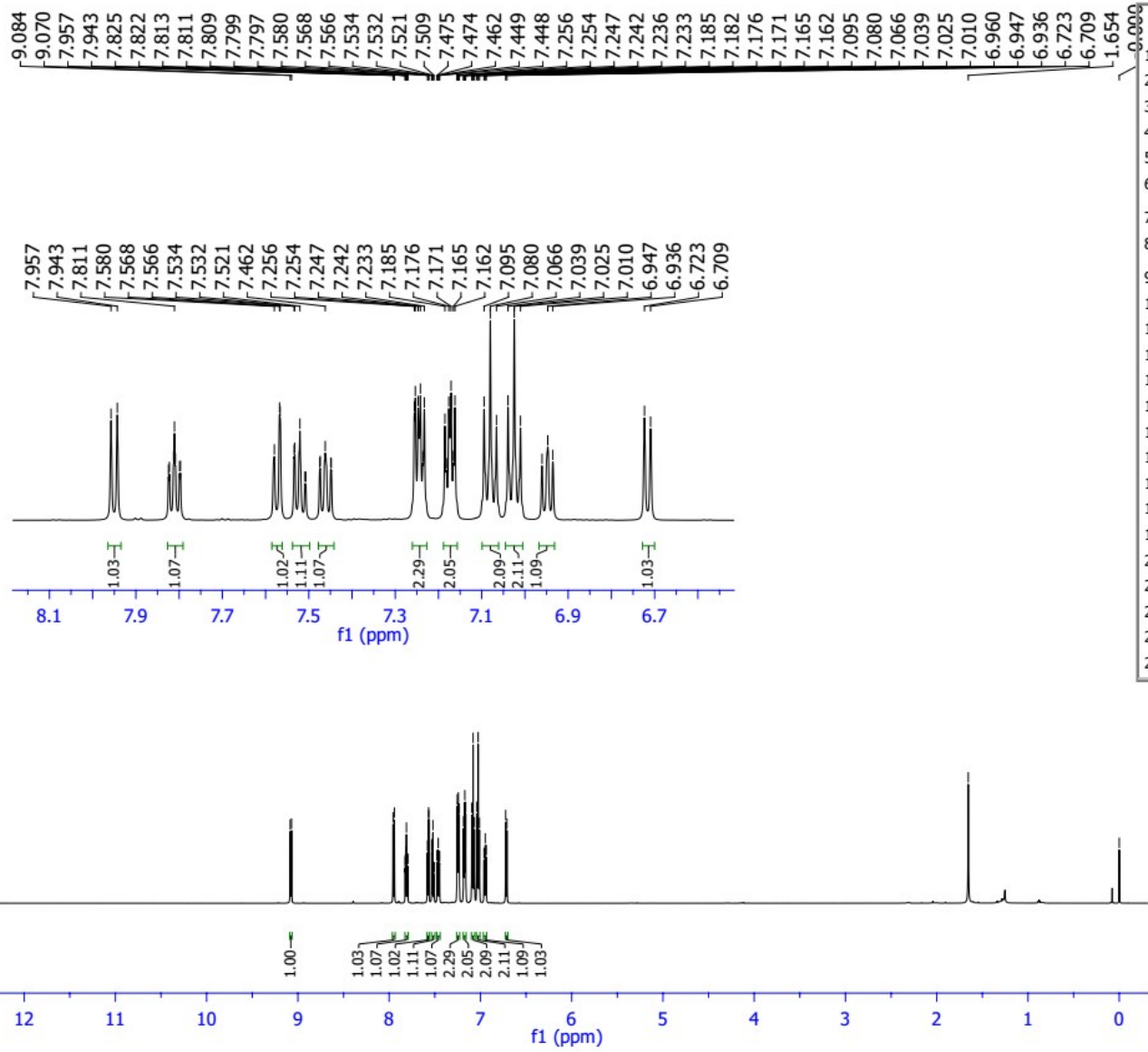


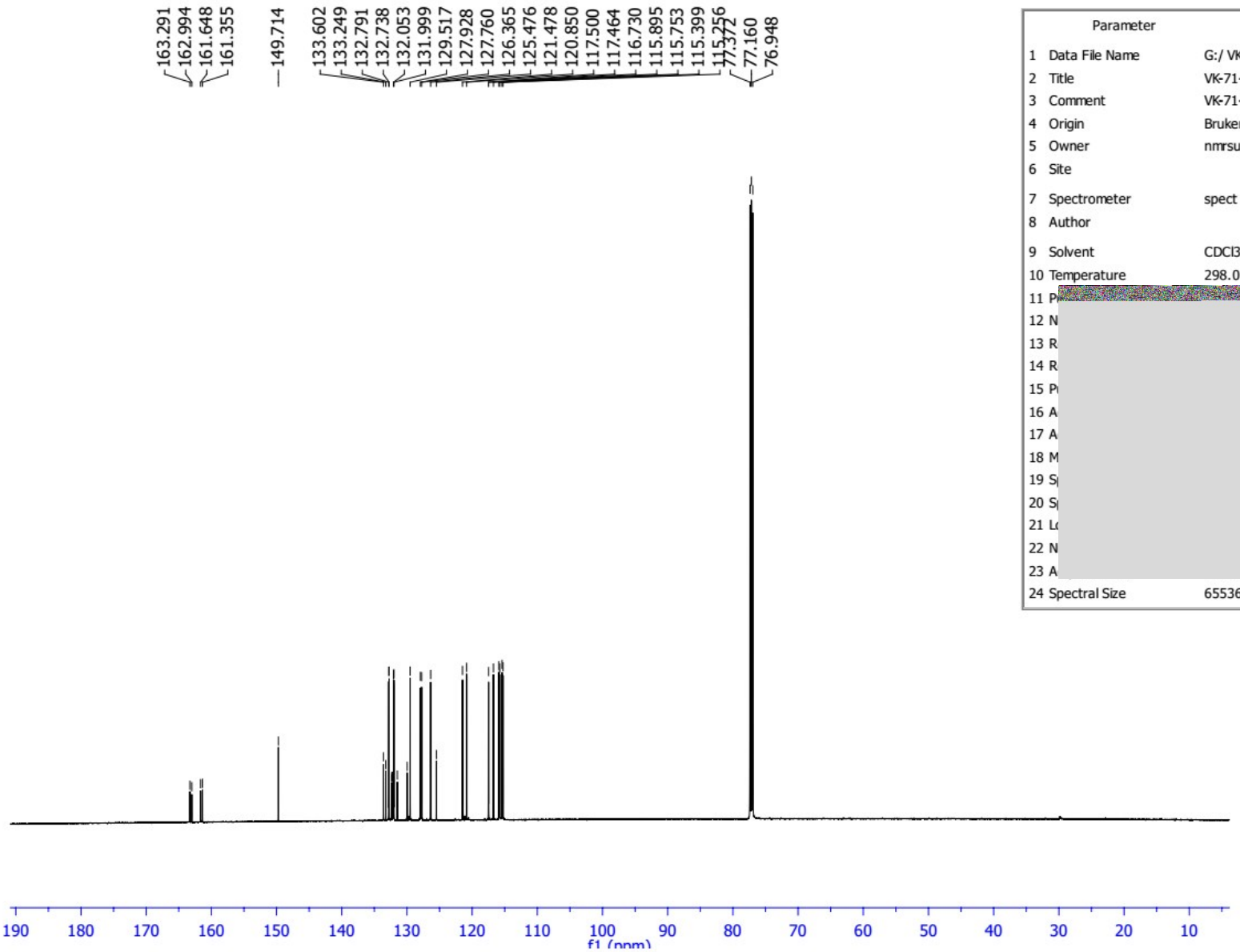
	Parameter	Value
1	Data File Name	C:/ Users/ VK-72A-1H/ 10/ fid
2	Title	VK-72A-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		
23	Acquired Size	32768
24	Spectral Size	65536





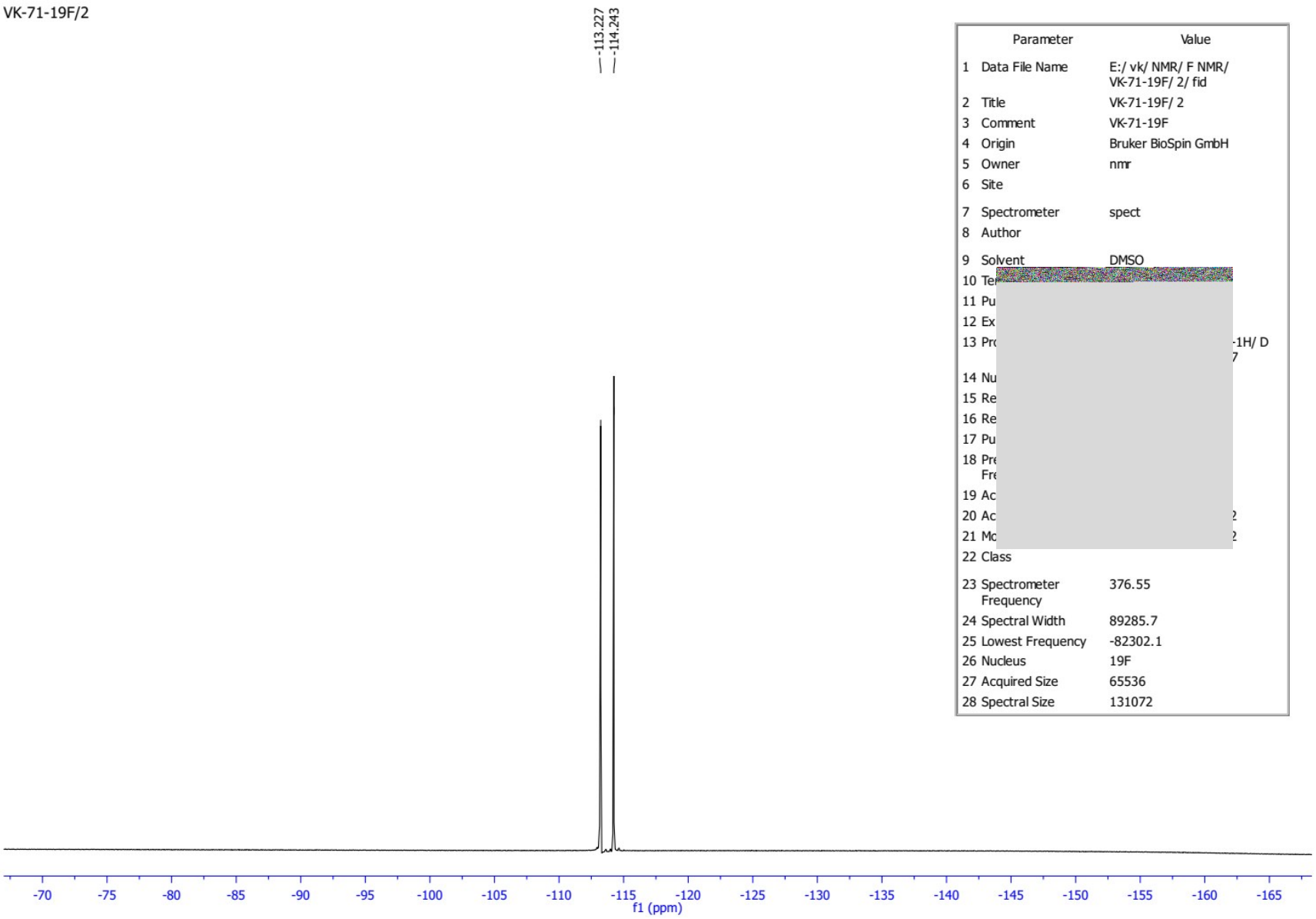
	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-72A-13C/ 10/ fid
2	Title	VK-72A-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10		
11		
12		
13		
14		
15		
16		
17		27
18		30
19		
20		
21		
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


9.084 9.070 7.957 7.943 7.825 7.822 7.813 7.811 7.809 7.799 7.797 7.580 7.568 7.566 7.534 7.532 7.521 7.509 7.475 7.474 7.462 7.449 7.448 7.256 7.254 7.247 7.242 7.236 7.233 7.185 7.182 7.176 7.171 7.165 7.162 7.095 7.080 7.066 7.039 7.025 7.010 6.960 6.947 6.936 6.723 6.709 1.654
7.957 7.943 7.811 7.580 7.568 7.566 7.534 7.532 7.521 7.462 7.256 7.254 7.247 7.242 7.233 7.185 7.176 7.171 7.165 7.162 7.095 7.080 7.066 7.039 7.025 7.010 6.947 6.936 6.723 6.709
1.03 1.07 1.02 1.11 1.07 2.29 2.05 2.09 2.11 1.09 1.03
8.1 7.9 7.7 7.5 7.3 7.1 6.9 6.7
f1 (ppm)
Parameter Value
1 Data File Name G:/ VK-71-1H/ 10/ fid
2 Title VK-71-1H
3 Comment VK-71-1H
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pu
12 Nu
13 Re
14 Re
15 Pu
16 Ac
17 Ac
18 Mc
19 Sp
20 Sp
21 Lo
22 Nu
23 Ac
24 Spectral Size 65536
F
F
N
N
3ad
3:00
3:14
1.00 1.03 1.07 1.02 1.11 1.07 2.29 2.05 2.09 2.11 1.09 1.03
12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

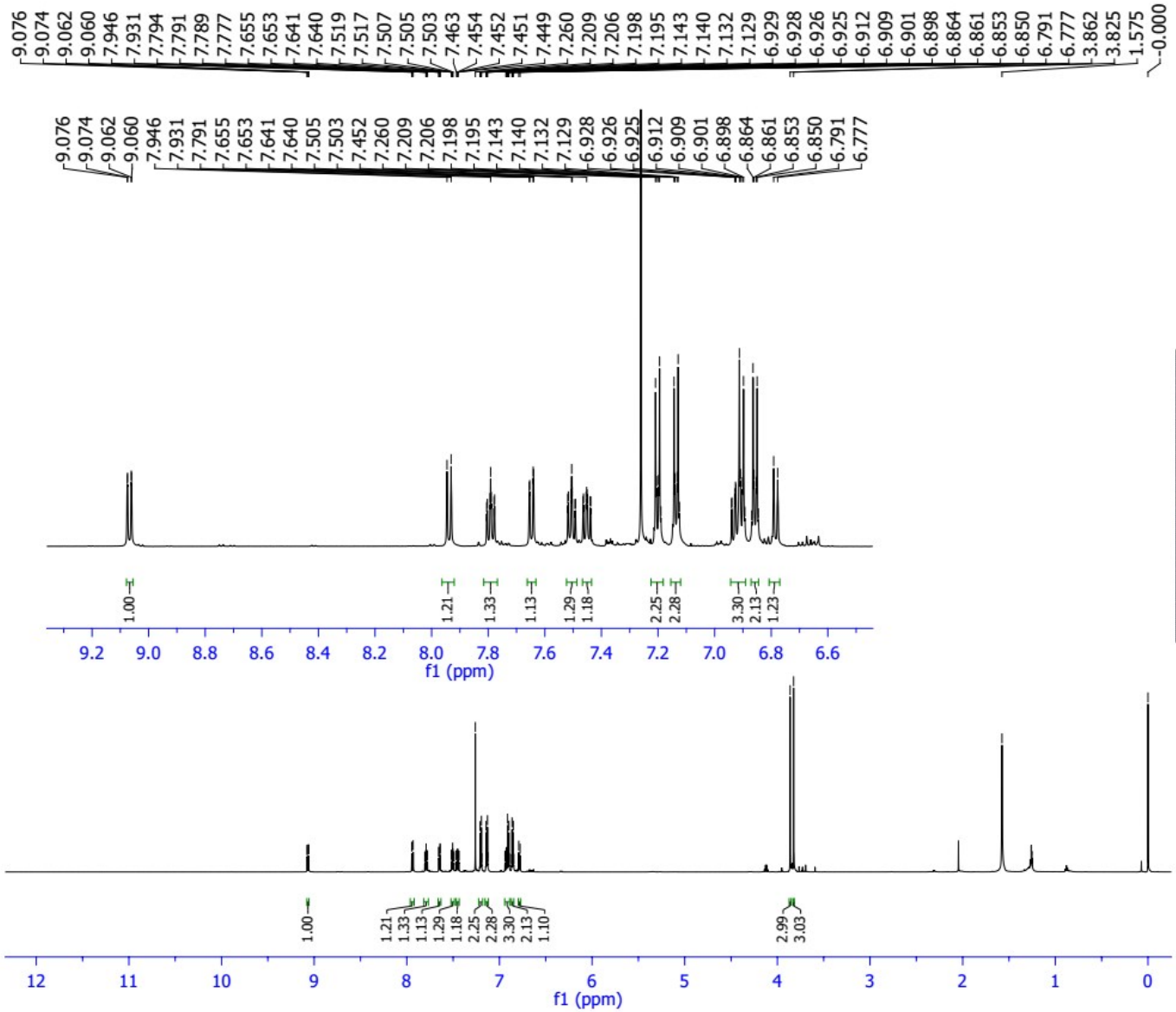


	Parameter	Value
1	Data File Name	G:/ VK-71-13C/ 10/ fid
2	Title	VK-71-13C
3	Comment	VK-71-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	P[redacted]	
12	N[redacted]	
13	R[redacted]	
14	R[redacted]	
15	P[redacted]	
16	A[redacted]	
17	A[redacted]	49:00
18	M[redacted]	49:04
19	S[redacted]	
20	S[redacted]	
21	L[redacted]	
22	N[redacted]	
23	A[redacted]	
24	Spectral Size	65536

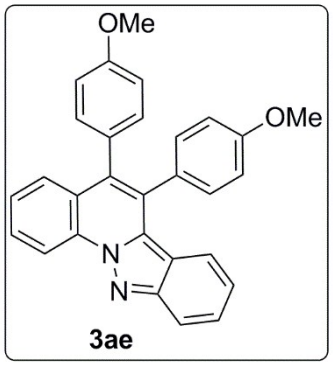
VK-71-19F/2



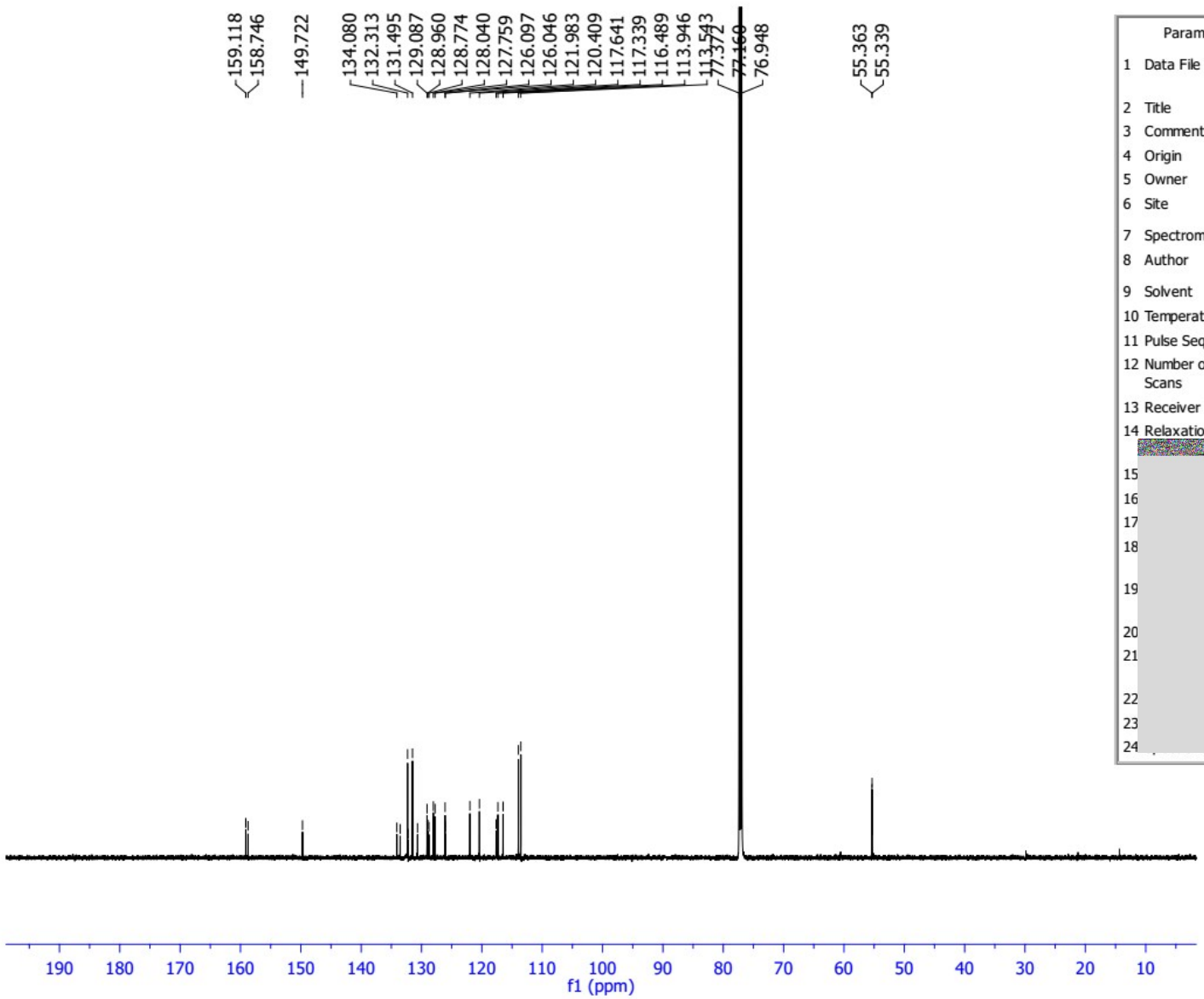
	Parameter	Value
1	Data File Name	E:/ vk/ NMR/ F NMR/ VK-71-19F/ 2/ fid
2	Title	VK-71-19F/ 2
3	Comment	VK-71-19F
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Te[redacted]	
11	Pu	
12	Ex	
13	Pr	-1H/ D 7
14	Nu	
15	Re	
16	Re	
17	Pu	
18	Pr Fr	
19	Ac	
20	Ac	2
21	Mc	2
22	Class	
23	Spectrometer Frequency	376.55
24	Spectral Width	89285.7
25	Lowest Frequency	-82302.1
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072



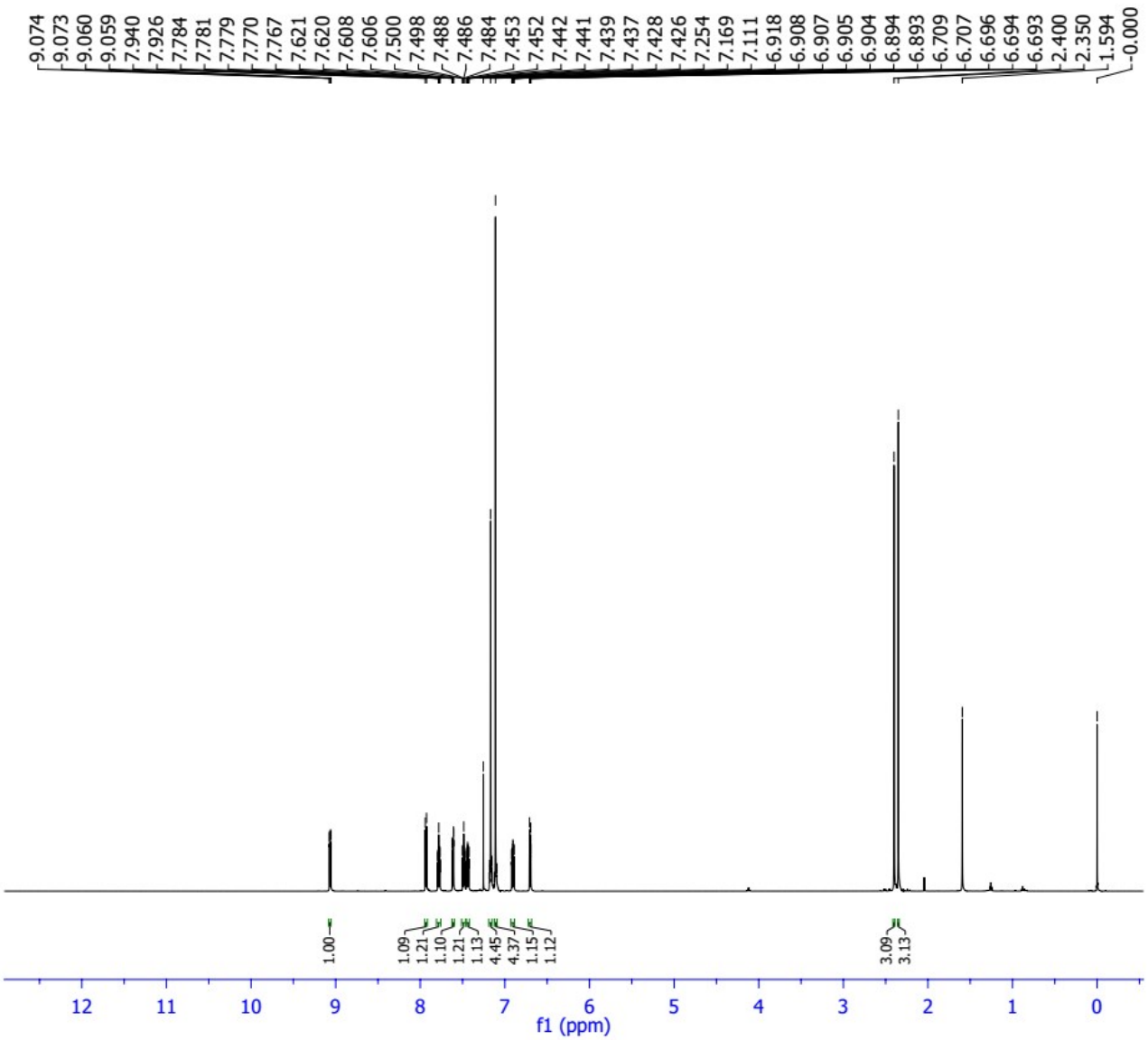
	Parameter	Value
1	Data File Name	H:/ NMR/ VK-75-1H/ 10/ fid
2	Title	VK-75-1H
3	Comment	VK-75-1H
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0



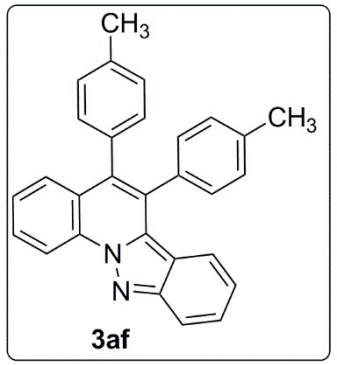
3ae

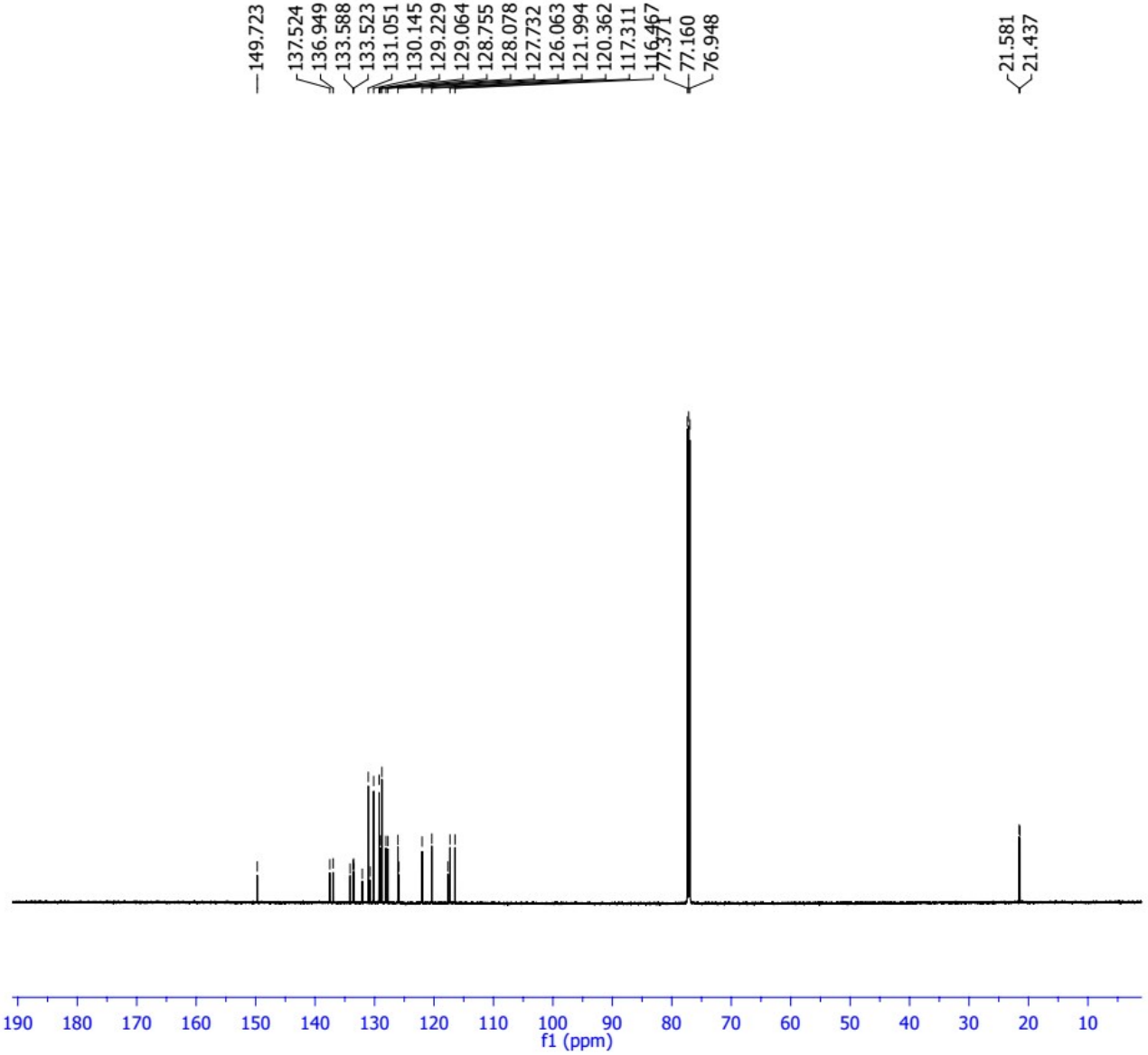


	Parameter	Value
1	Data File Name	H:/ NMR/ VK-75-13C/ 10/ fid
2	Title	VK-75-13C
3	Comment	VK-75-13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	500
13	Receiver Gain	200
14	Relaxation	2.0000
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		

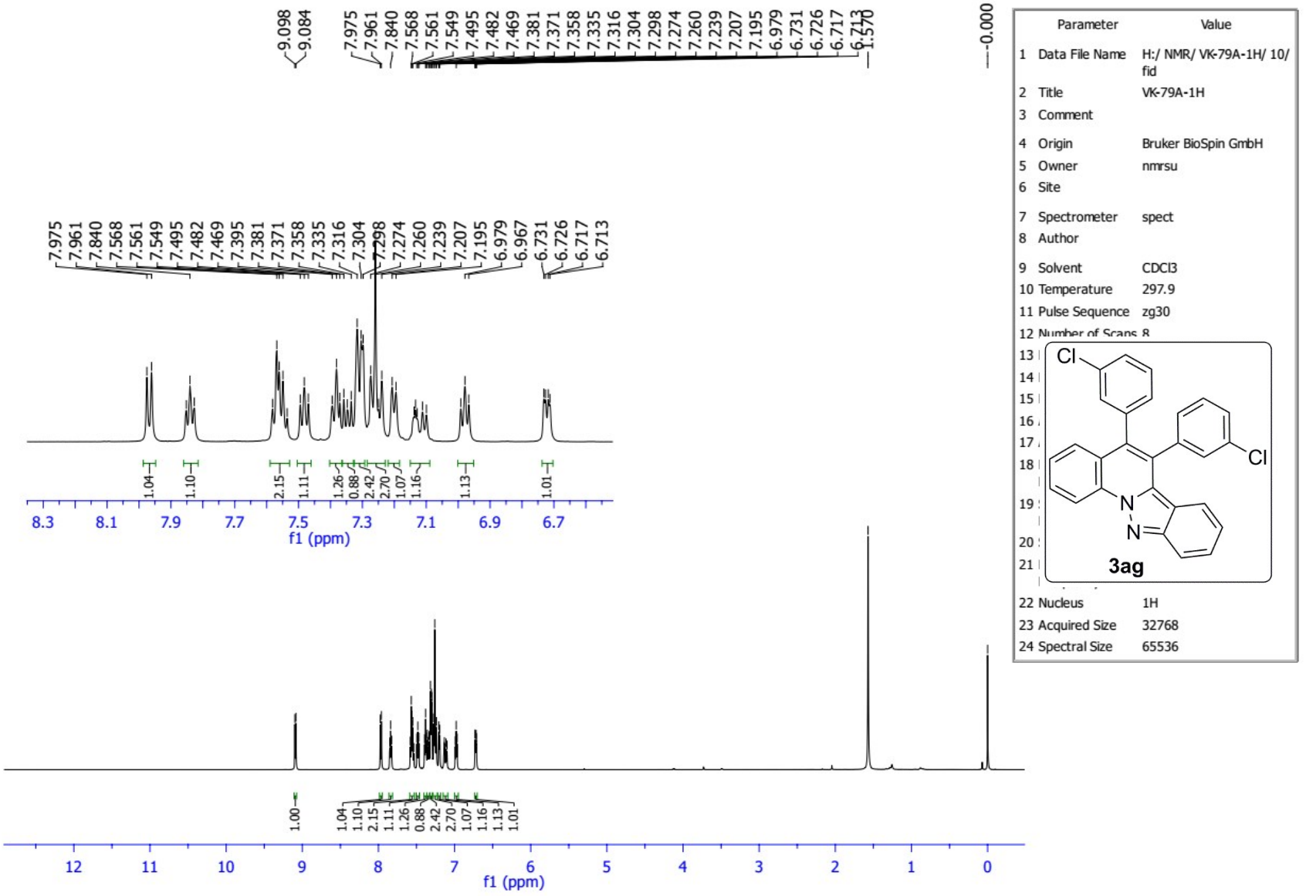


	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-SV-31-10-17/ VK-74-1H/ 10/ fid
2	Title	VK-74-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21	Lowest Frequency	-2321.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536





	Parameter	Value
1	Data File Name	C:/ Users/ T Punniyamurthy/ Desktop/ VK-SV-31-10-17/ VK-74-13C/ 10/ fid
2	Title	VK-74-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	N	
13	R	
14	R	
15	P	
16	A	
17	A	
18	M	
19	S F	
20	S	
21	L F	
22	N	
23	Acquired Size	32768
24	Spectral Size	65536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9.084
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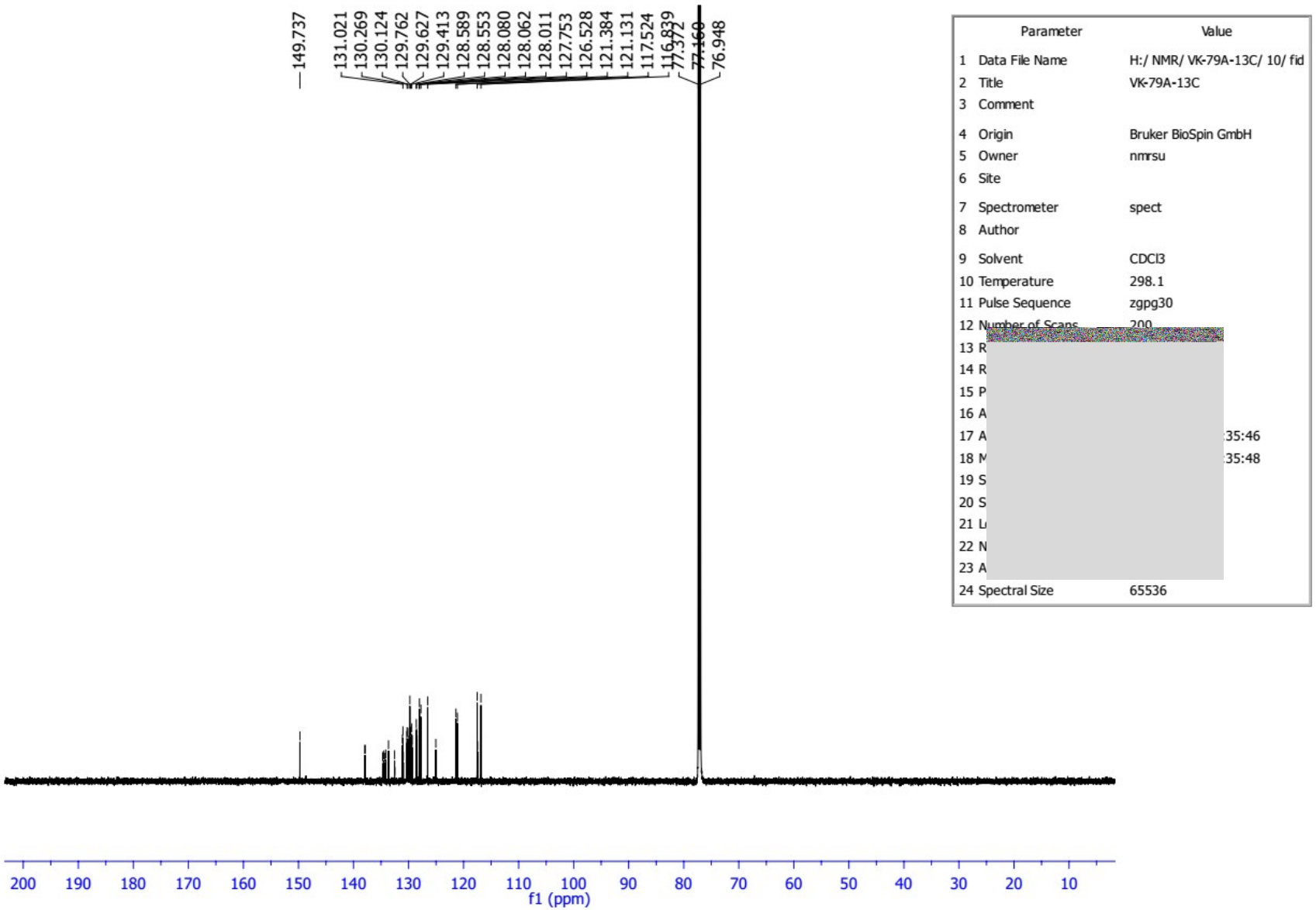
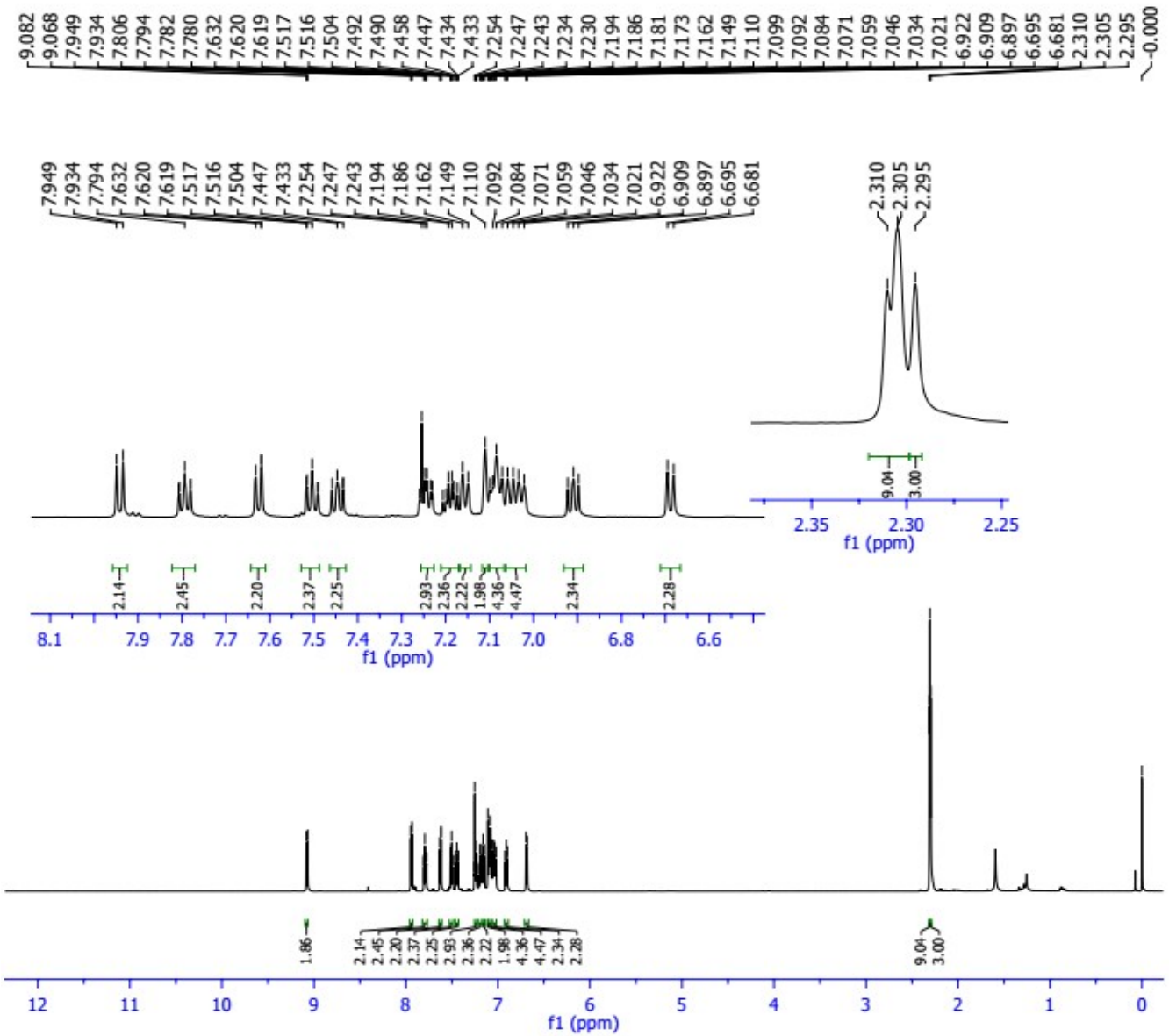
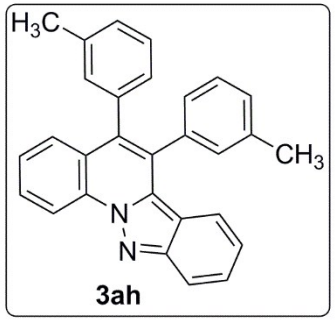
7.561
7.549
7.495
7.482
7.469
7.381
7.371
7.358
7.335
7.316
7.304
7.298
7.274
7.260
7.239
7.207
7.195
6.979
6.731
6.726
6.717
6.713
1.570
0.000
1.04
1.10
2.15
1.11
1.26
0.88
2.42
2.70
1.07
1.16
1.13
1.01
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
1.00
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)
Parameter
Value
1 Data File Name
H:/ NMR/ VK-79A-1H/ 10/ fid
2 Title
VK-79A-1H
3 Comment
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Author
9 Solvent
CDCl3
10 Temperature
297.9
11 Pulse Sequence
zg30
12 Number of Scans 8
Cl
Cl
N
N
3ag
22 Nucleus
1H
23 Acquired Size
32768
24 Spectral Size
65536



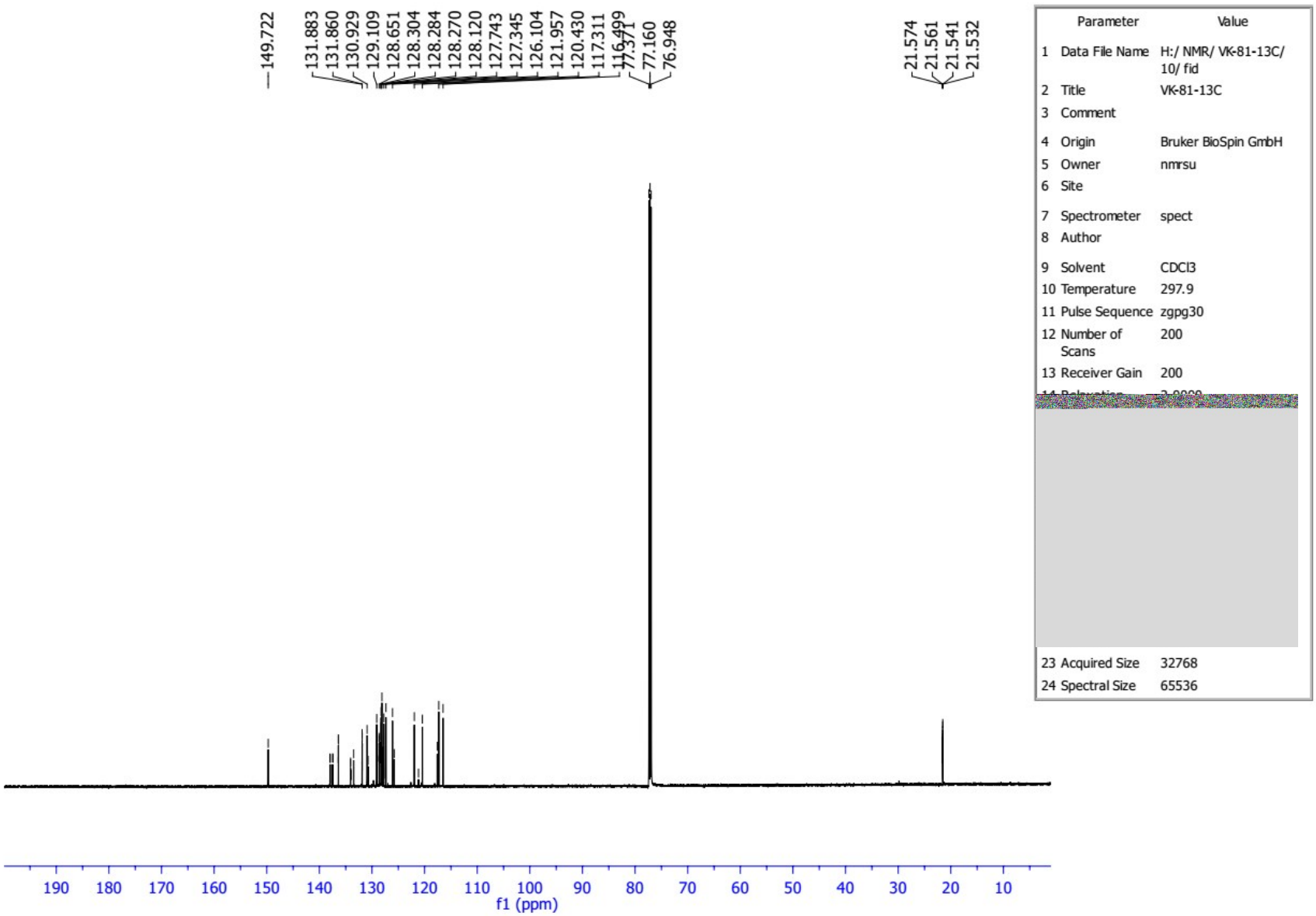
	Parameter	Value
1	Data File Name	H:/ NMR/ VK-79A-13C/ 10/ fid
2	Title	VK-79A-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Number of Scans	200
13	R	
14	R	
15	P	
16	A	
17	A	35:46
18	M	35:48
19	S	
20	S	
21	L	
22	N	
23	A	
24	Spectral Size	65536



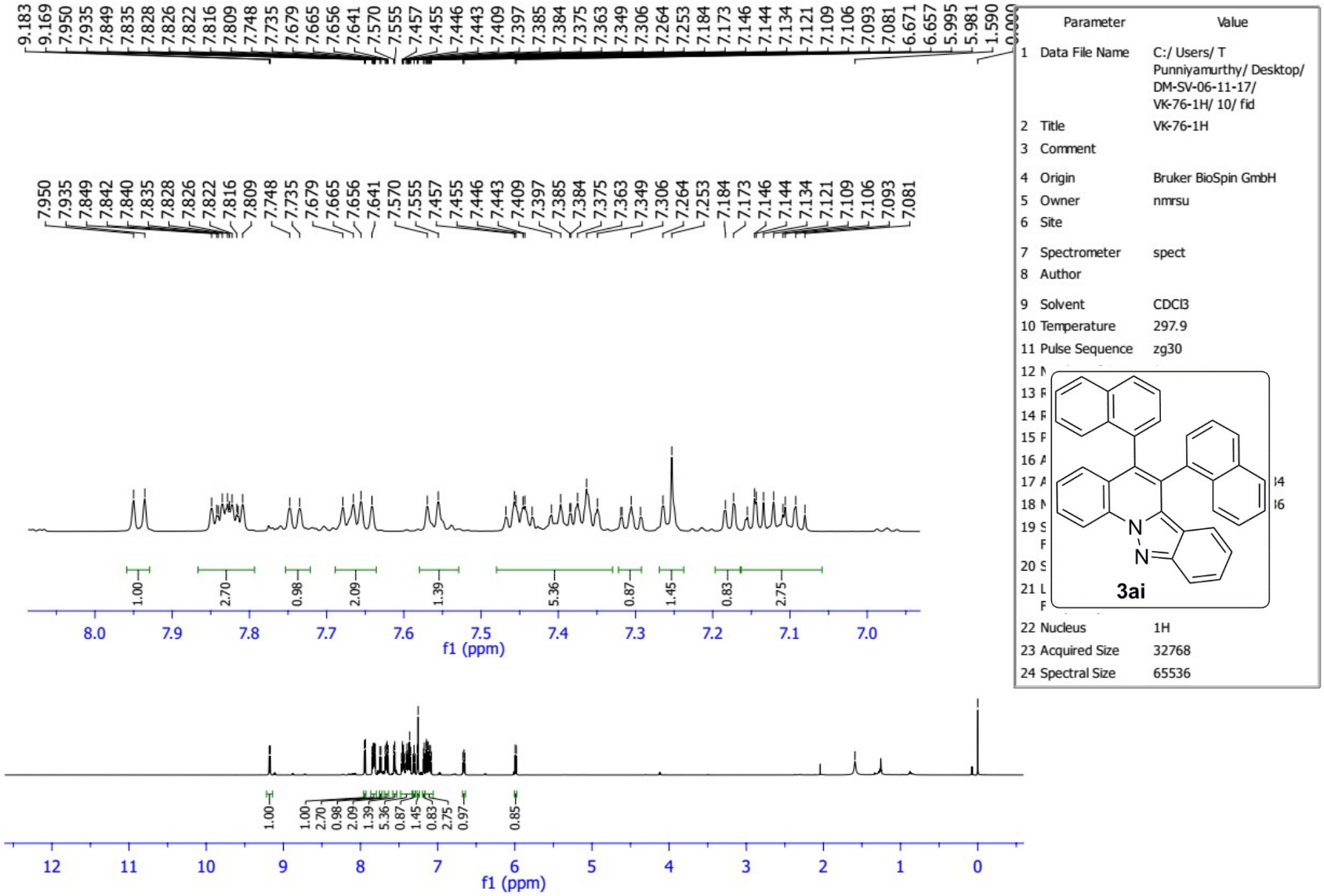
	Parameter	Value
1	Data File Name	H:/ NMR/ VK-81-1H/ 10/ fid
2	Title	VK-81-1H
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30

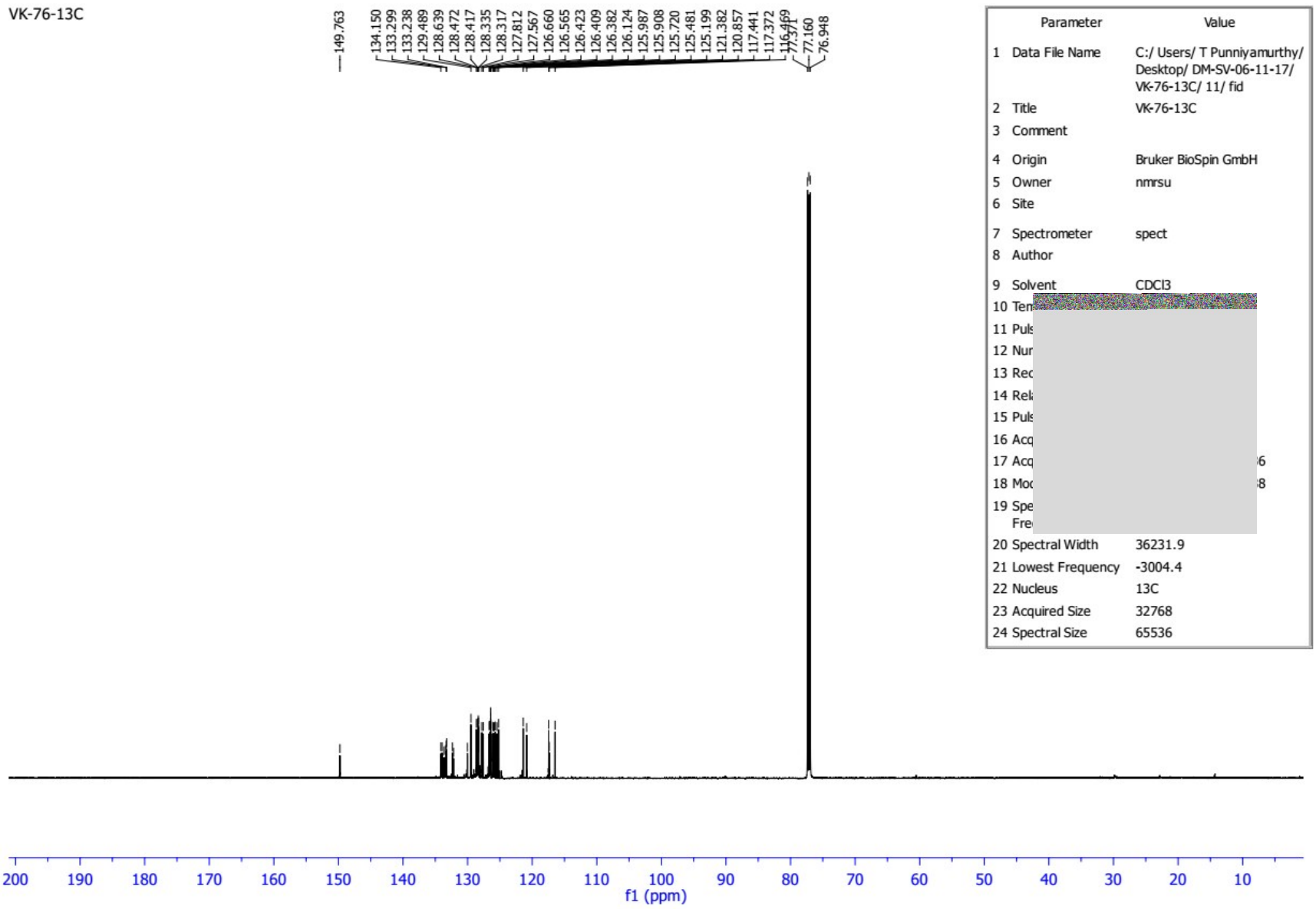


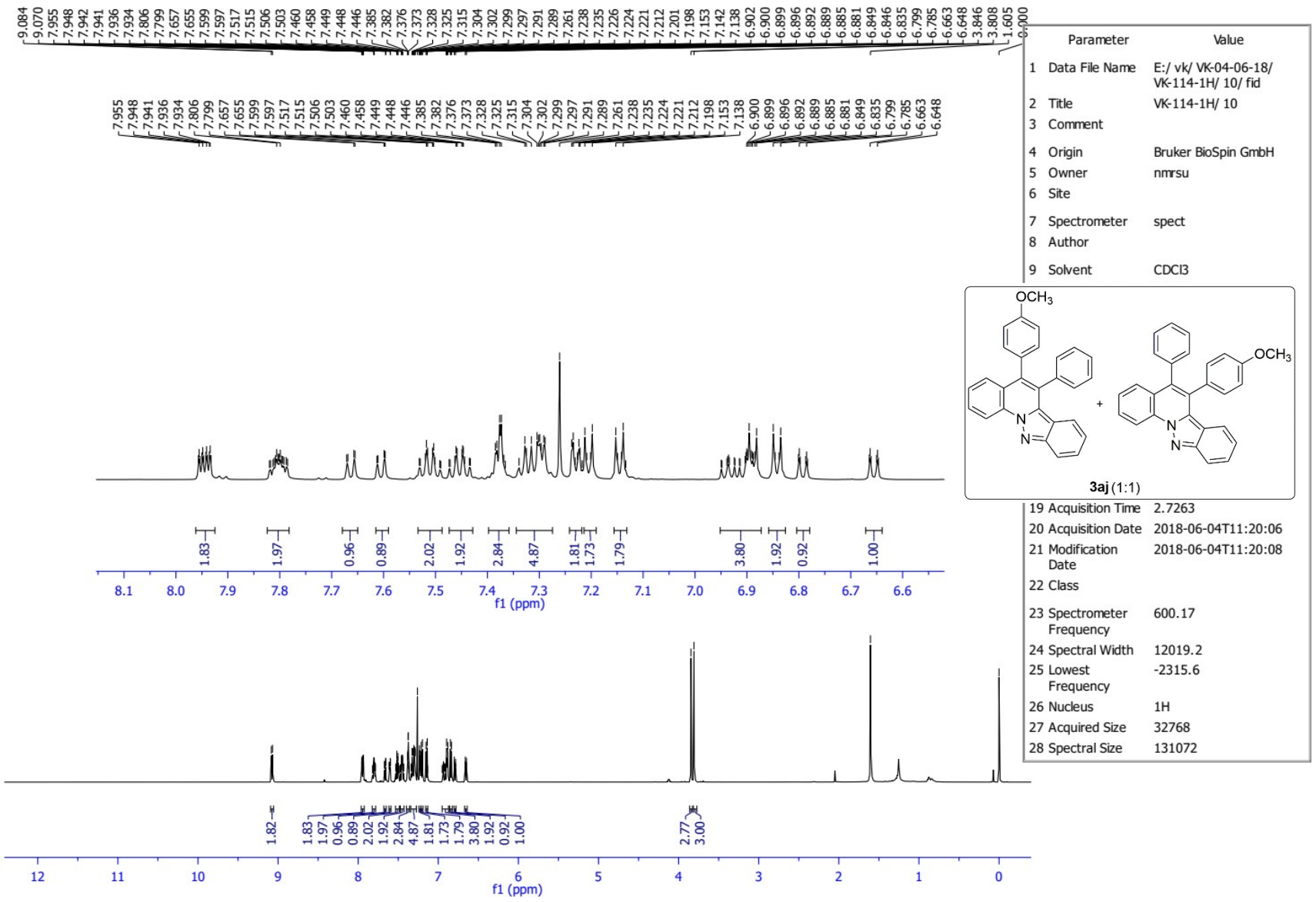
Frequency



	Parameter	Value
1	Data File Name	H:/ NMR/ VK-81-13C/ 10/ fid
2	Title	VK-81-13C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Number of Scans	200
13	Receiver Gain	200
23	Acquired Size	32768
24	Spectral Size	65536


9.183 9.169 7.950 7.935 7.849 7.835 7.828 7.826 7.822 7.816 7.809 7.748 7.735 7.679 7.665 7.656 7.641 7.570 7.555 7.457 7.455 7.446 7.443 7.409 7.397 7.385 7.384 7.375 7.363 7.349 7.306 7.264 7.253 7.184 7.173 7.146 7.144 7.134 7.121 7.109 7.106 7.093 7.081 6.671 6.657 5.995 5.981 1.590
7.950 7.935 7.849 7.842 7.840 7.835 7.828 7.826 7.822 7.816 7.809 7.748 7.735 7.679 7.665 7.656 7.641 7.570 7.555 7.457 7.455 7.446 7.443 7.409 7.397 7.385 7.384 7.375 7.363 7.349 7.306 7.264 7.253 7.184 7.173 7.146 7.144 7.134 7.121 7.109 7.106 7.093 7.081
1.00 2.70 0.98 2.09 1.39 5.36 0.87 1.45 0.83 2.75
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
1.00 1.00 2.70 0.98 2.09 1.39 5.36 0.87 1.45 0.83 2.75 0.97 0.85
12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
Parameter Value
1 Data File Name C:/ Users/ T Punniyamurthy/ Desktop/ DM-SV-06-11-17/ VK-76-1H/ 10/ fid
2 Title VK-76-1H
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 297.9
11 Pulse Sequence zg30
22 Nucleus 1H
23 Acquired Size 32768
24 Spectral Size 65536
N
N
3ai


VK-76-13C
149.763
134.150
133.299
133.238
129.489
128.639
128.472
128.417
128.335
128.317
127.812
127.567
126.660
126.565
126.423
126.409
126.382
126.124
125.987
125.908
125.720
125.481
125.199
121.382
120.857
117.441
117.372
116.469
77.371
77.160
76.948
Parameter Value
1 Data File Name C:/ Users/ T Punniyamurthy/ Desktop/ DM-SV-06-11-17/ VK-76-13C/ 11/ fid
2 Title VK-76-13C
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
20 Spectral Width 36231.9
21 Lowest Frequency -3004.4
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


9.084 9.070 7.955 7.948 7.942 7.941 7.936 7.934 7.806 7.799 7.657 7.655 7.599 7.597 7.517 7.515 7.506 7.503 7.460 7.458 7.449 7.448 7.446 7.385 7.382 7.376 7.373 7.328 7.325 7.315 7.304 7.302 7.299 7.297 7.291 7.289 7.261 7.238 7.235 7.226 7.224 7.221 7.212 7.201 7.198 7.153 7.142 7.138 6.902 6.900 6.899 6.896 6.892 6.889 6.885 6.881 6.849 6.846 6.835 6.799 6.785 6.663 6.648 3.846 3.808 1.605 0.000
7.955 7.948 7.941 7.936 7.934 7.806 7.799 7.657 7.655 7.599 7.597 7.517 7.515 7.506 7.503 7.460 7.458 7.449 7.448 7.446 7.385 7.382 7.376 7.373 7.328 7.325 7.315 7.304 7.302 7.299 7.297 7.291 7.289 7.261 7.238 7.235 7.224 7.221 7.212 7.198 7.153 7.138 6.900 6.899 6.896 6.892 6.889 6.885 6.881 6.849 6.835 6.799 6.785 6.663 6.648
1.83 1.97 0.96 0.89 2.02 1.92 2.84 4.87 1.81 1.73 1.79 3.80 1.92 0.92 1.00
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
f1 (ppm)
1.82 1.83 1.97 0.96 0.89 2.02 1.92 2.84 4.87 1.81 1.73 1.79 3.80 1.92 0.92 1.00 2.77 3.00
12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
Parameter Value
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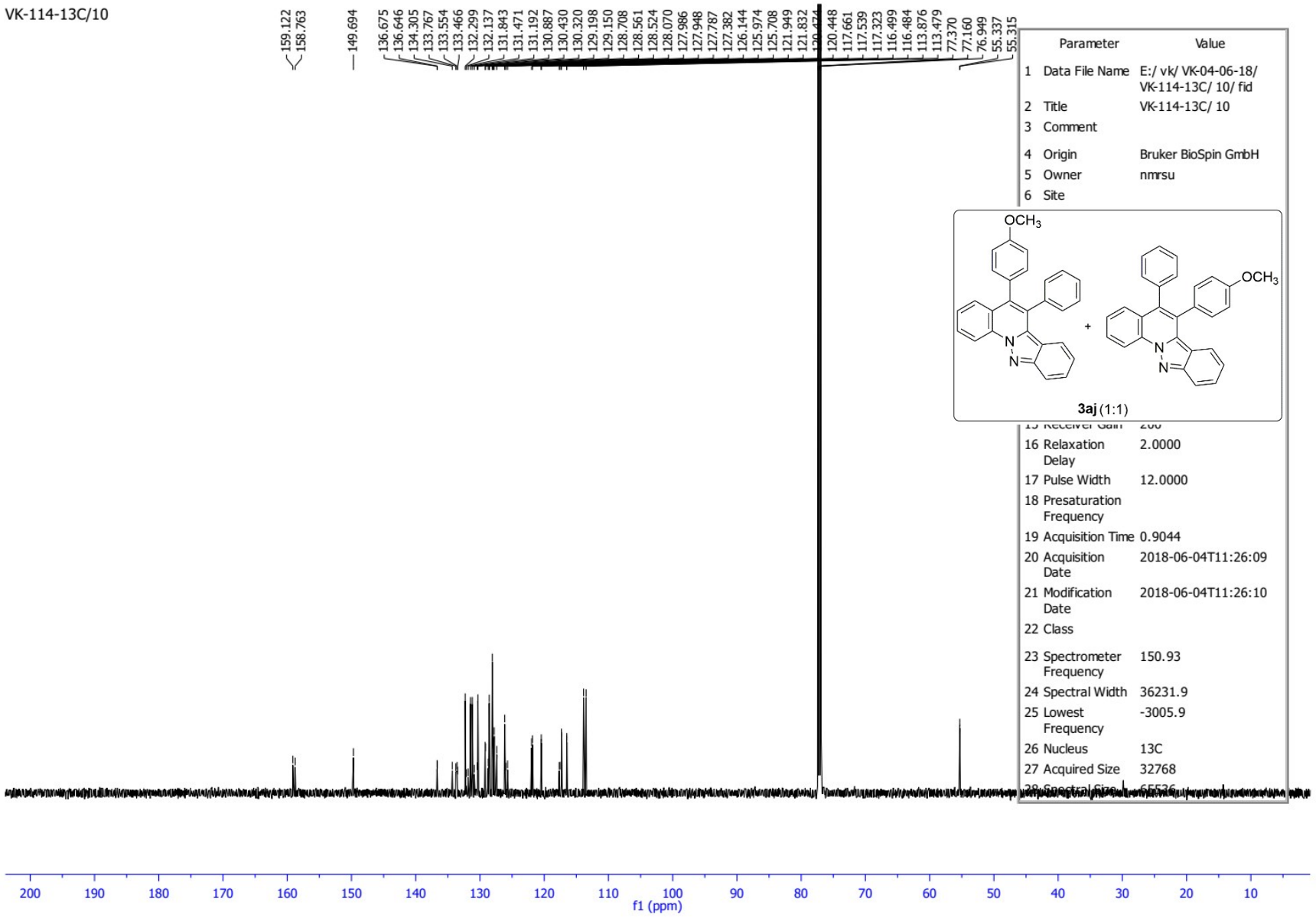
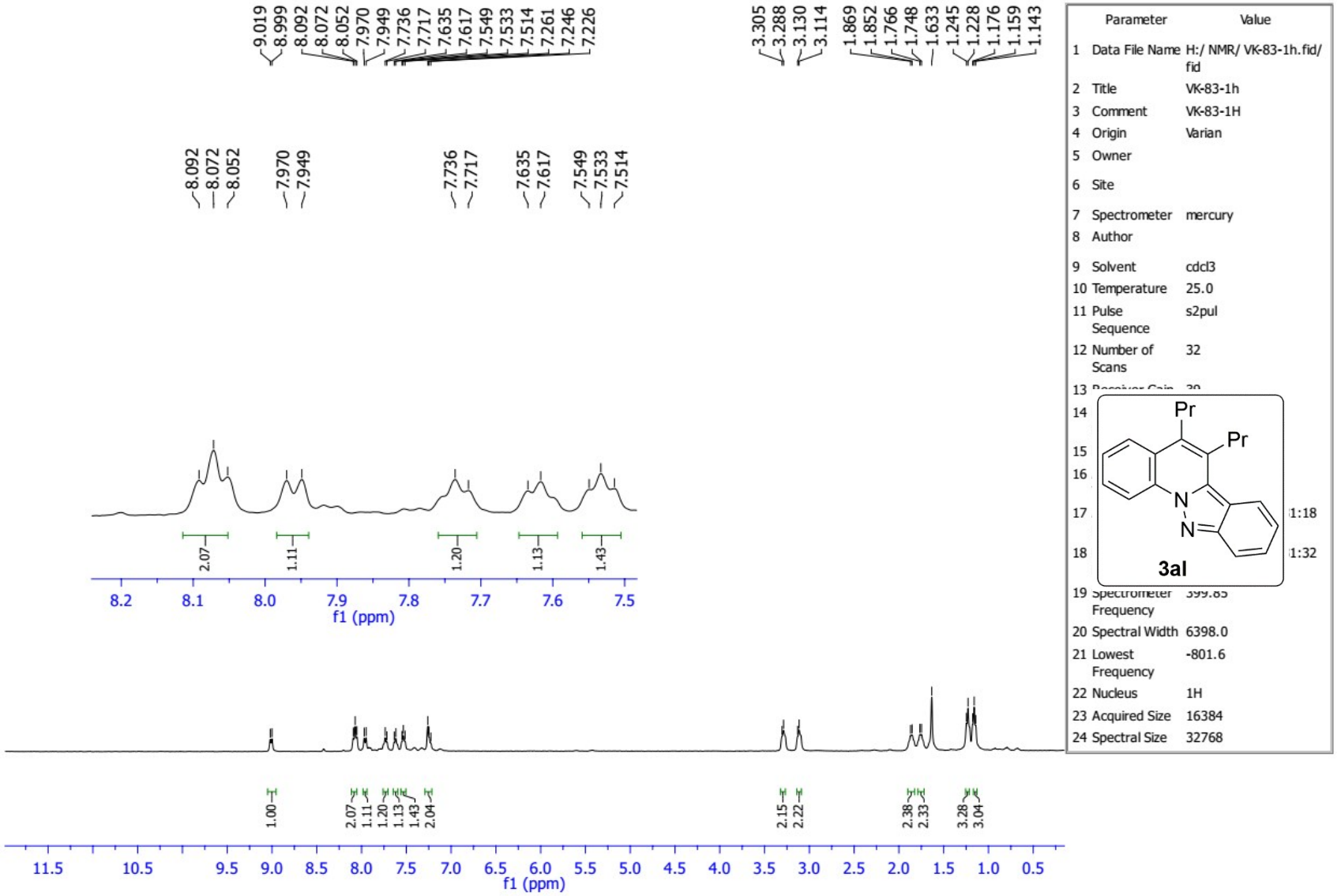
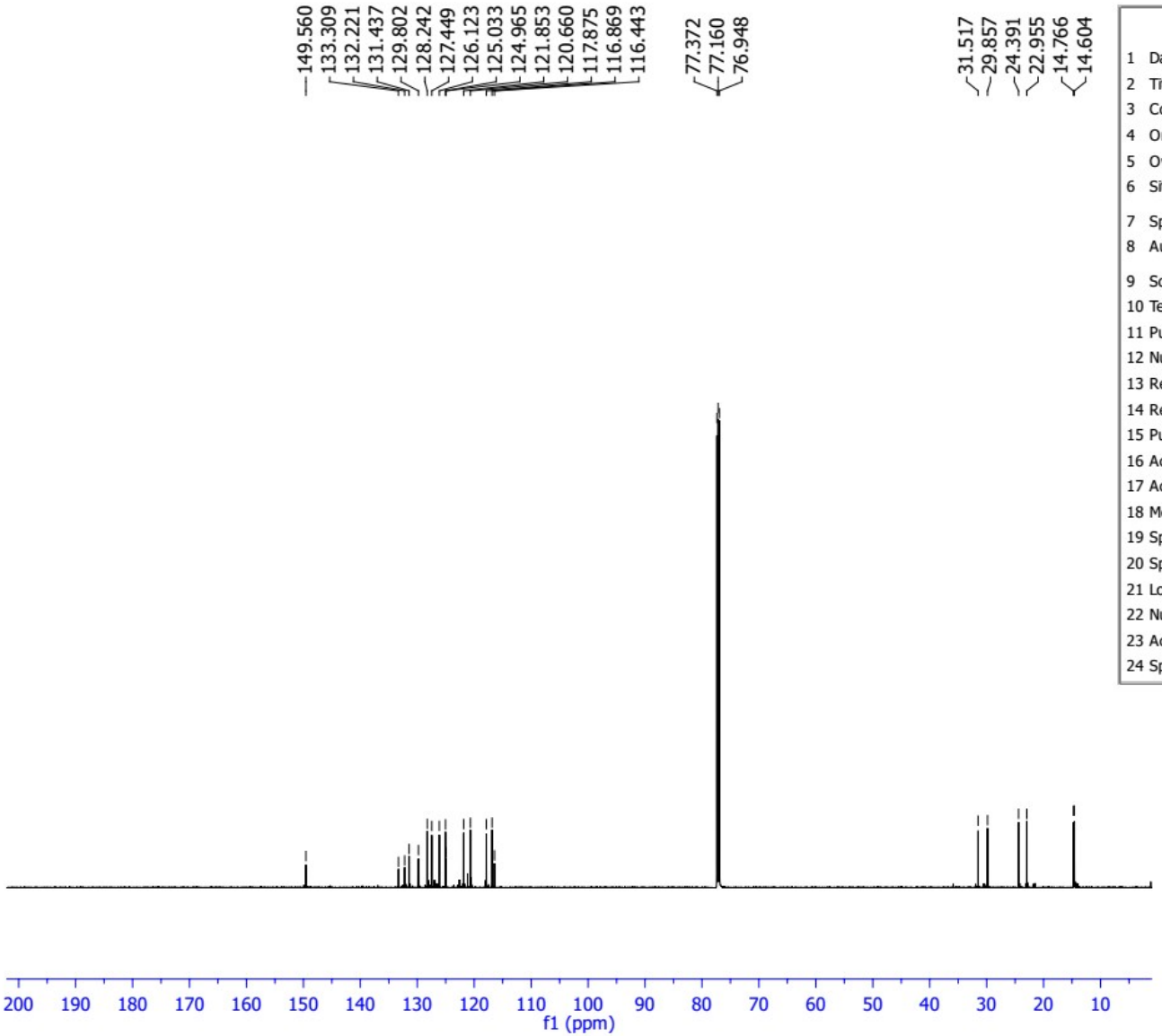
2 Title VK-114-1H/ 10
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
OCH3
OCH3
3aj (1:1)
19 Acquisition Time 2.7263
20 Acquisition Date 2018-06-04T11:20:06
21 Modification Date 2018-06-04T11:20:08
22 Class
23 Spectrometer Frequency 600.17
24 Spectral Width 12019.2
25 Lowest Frequency -2315.6
26 Nucleus 1H
27 Acquired Size 32768
28 Spectral Size 131072

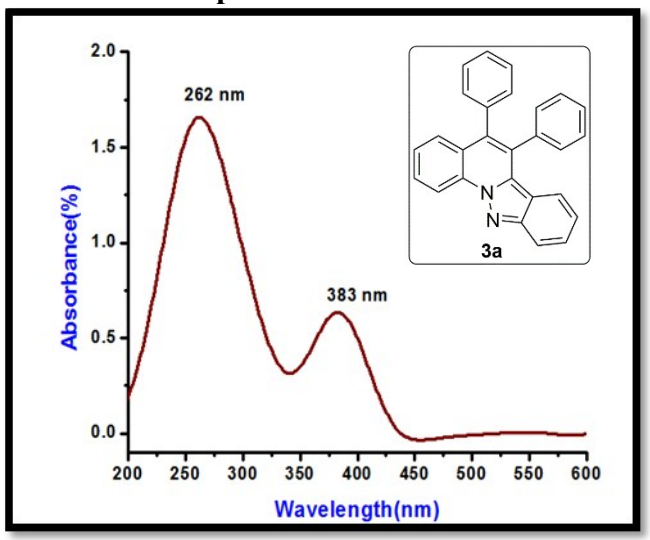

VK-114-13C/10
159.122
158.763
149.694
136.675
136.646
134.305
133.767
133.554
133.466
132.299
132.137
131.843
131.471
131.192
130.887
130.430
130.320
129.198
129.150
128.708
128.561
128.524
128.070
127.986
127.948
127.787
127.382
126.144
125.974
125.708
121.949
121.832
120.448
117.661
117.539
117.323
116.499
116.484
113.876
113.479
77.370
77.160
76.949
55.337
55.315
Parameter Value
1 Data File Name E:/ vk/ VK-04-06-18/ VK-114-13C/ 10/ fid
2 Title VK-114-13C/ 10
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
OCH3
OCH3
3aj (1:1)
16 Relaxation Delay 2.0000
17 Pulse Width 12.0000
18 Presaturation Frequency
19 Acquisition Time 0.9044
20 Acquisition Date 2018-06-04T11:26:09
21 Modification Date 2018-06-04T11:26:10
22 Class
23 Spectrometer Frequency 150.93
24 Spectral Width 36231.9
25 Lowest Frequency -3005.9
26 Nucleus 13C
27 Acquired Size 32768
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

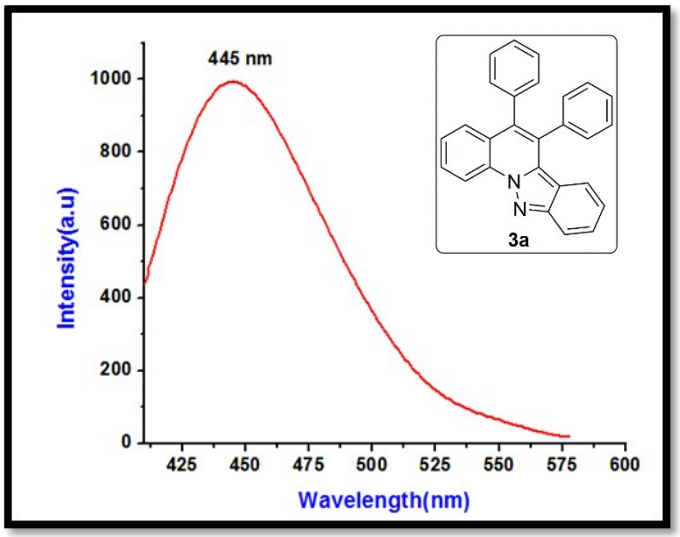

9.019
8.999
8.092
8.072
8.052
7.970
7.949
7.736
7.717
7.635
7.617
7.549
7.533
7.514
7.261
7.246
7.226
3.305
3.288
3.130
3.114
1.869
1.852
1.766
1.748
1.633
1.245
1.228
1.176
1.159
1.143
2.07
1.11
1.20
1.13
1.43
f1 (ppm)
1.00
2.07
1.11
1.20
1.13
1.43
2.04
2.15
2.22
2.38
2.33
3.28
3.04
f1 (ppm)
Parameter
Value
1 Data File Name H:/ NMR/ VK-83-1h.fid/ fid
2 Title VK-83-1h
3 Comment VK-83-1H
4 Origin Varian
5 Owner
6 Site
7 Spectrometer mercury
8 Author
9 Solvent cdcl3
10 Temperature 25.0
11 Pulse Sequence s2pul
12 Number of Scans 32
19 Frequency
20 Spectral Width 6398.0
21 Lowest Frequency -801.6
22 Nucleus 1H
23 Acquired Size 16384
24 Spectral Size 32768
Pr
Pr
N
N
3al
1:18
1:32

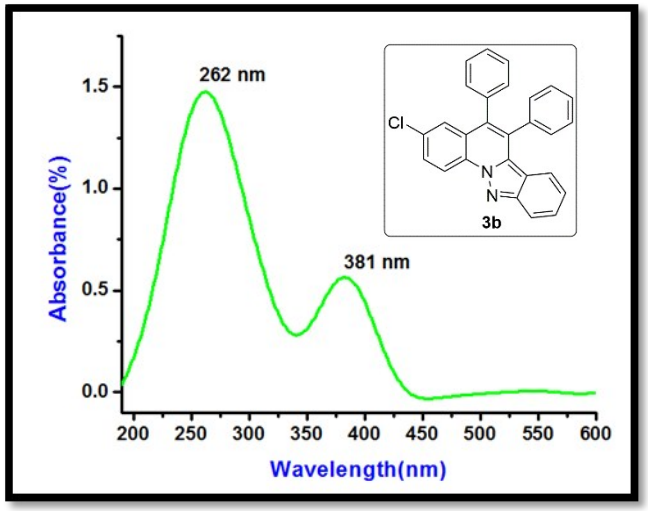


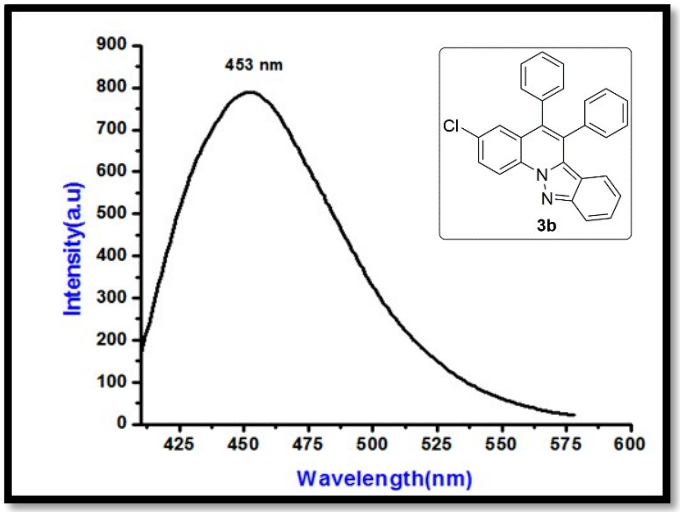
	Parameter	Value
1	Data File Name	H:/ NMR/ VK-83_13C/ 10/ fid
2	Title	VK-83_13C
3	Comment	VK-83_13C
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	500
13	Receiver Gain	200
14	Relaxa	
15	Pulse W	
16	Acquisit	
17	Acquisit	2:51:24
18	Modifica	2:51:26
19	Spectro	
20	Spectra	
21	Lowest	
22	Nucleus	
23	Acquired Size	32768
24	Spectral Size	65536

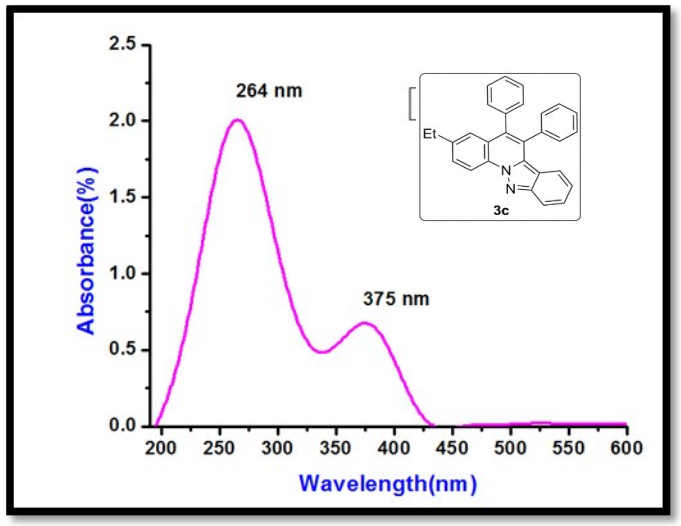
UV-Vis and Emission Spectra

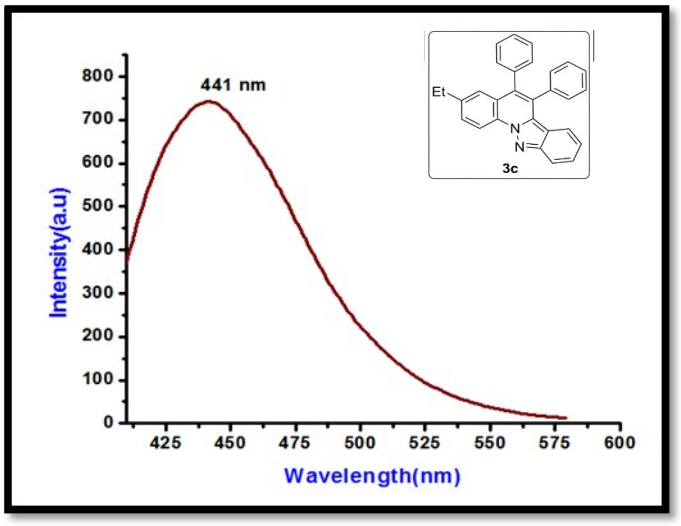


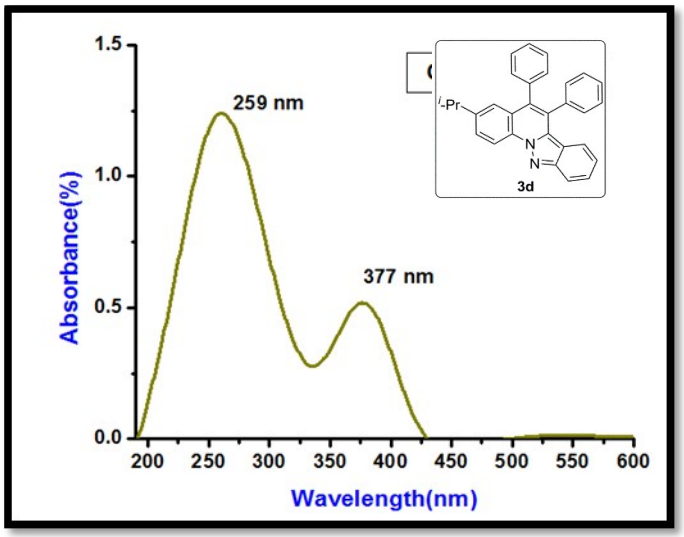


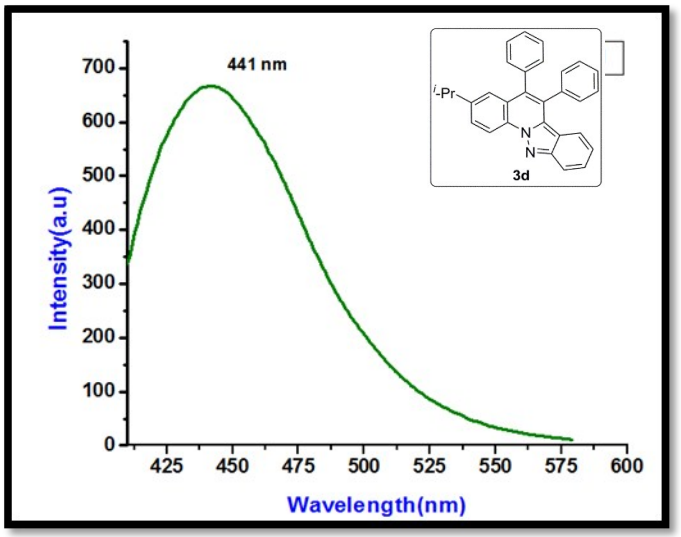


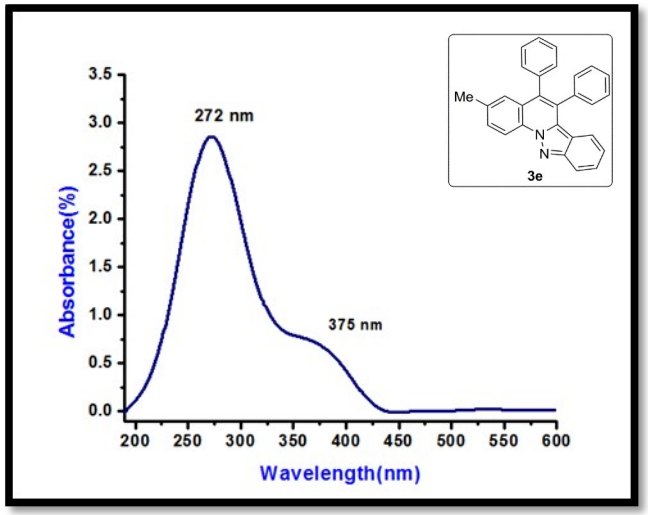


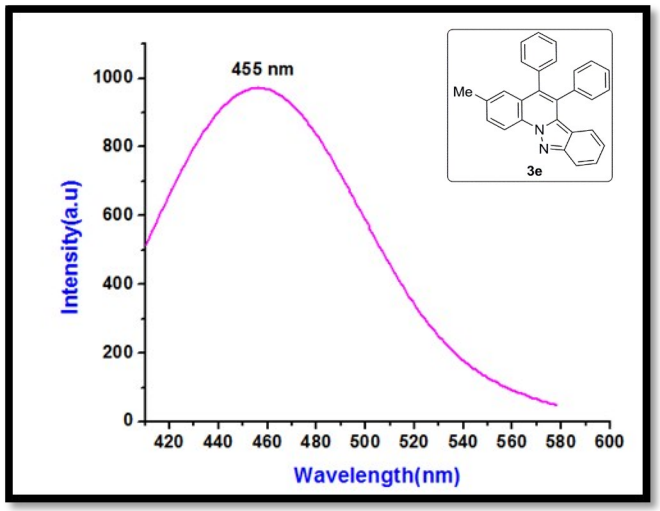

264 nm
375 nm
Absorbance(%)
Wavelength(nm)
Et
3c

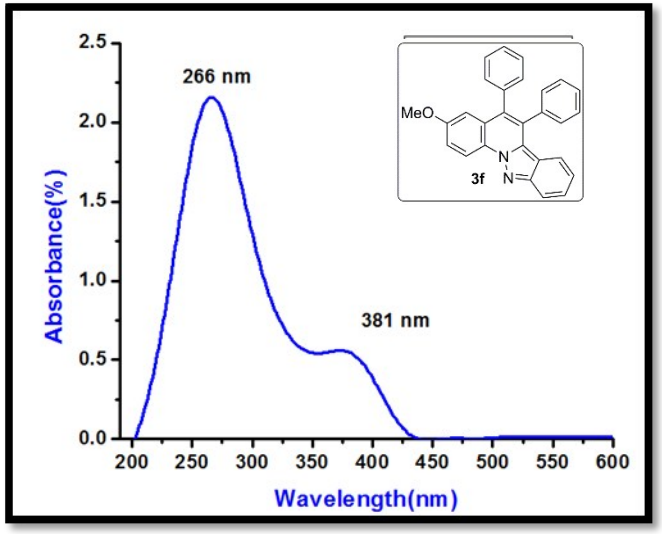

441 nm
Intensity(a.u)
Wavelength(nm)
Et
3c

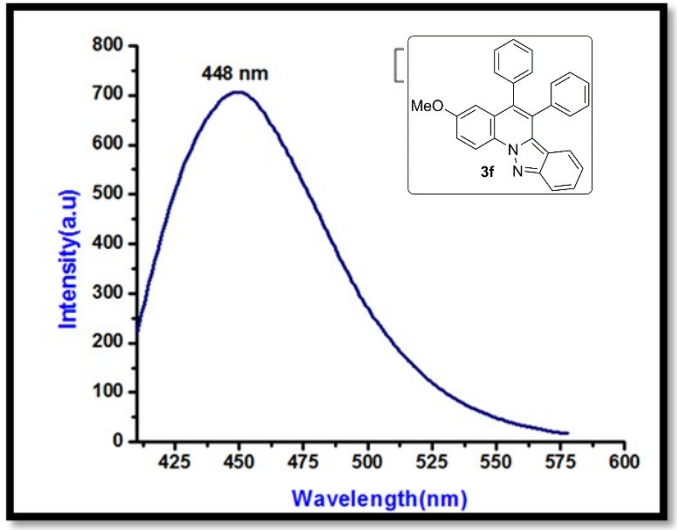

259 nm
377 nm
Absorbance(%)
Wavelength(nm)
i-Pr
3d

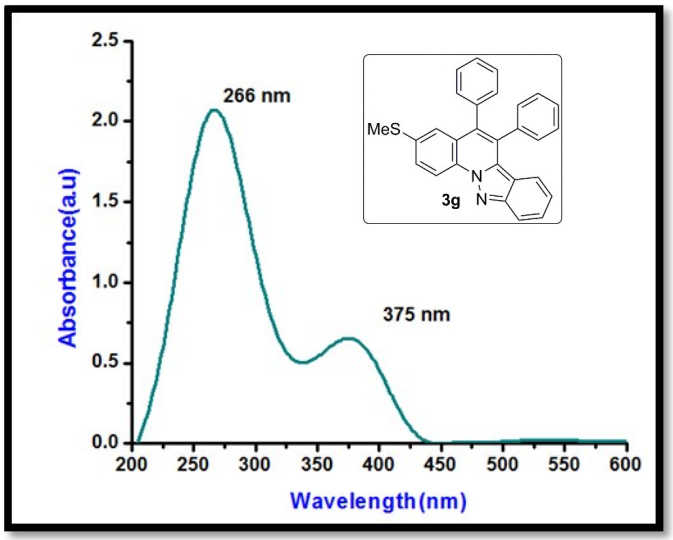

441 nm
Intensity(a.u)
Wavelength(nm)
i-Pr
3d

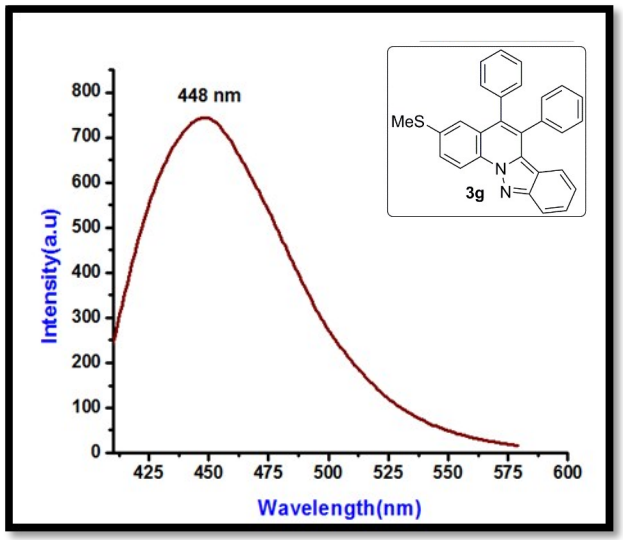

272 nm
375 nm
Absorbance(%)
Wavelength(nm)
Me
N
N
3e

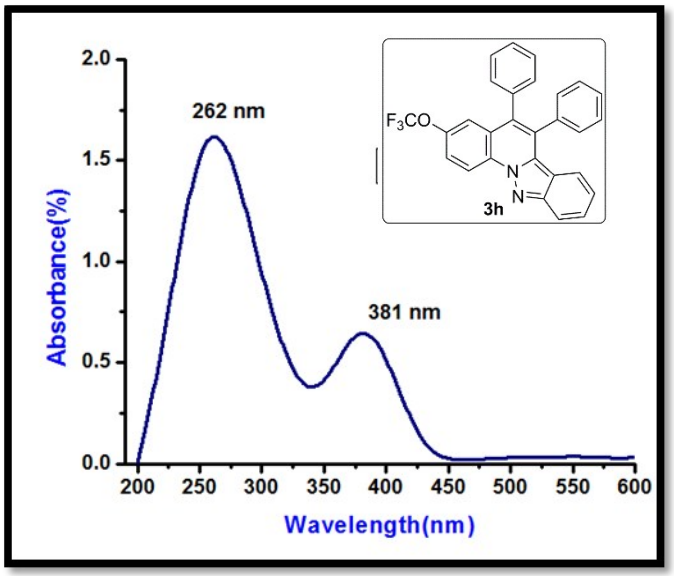

455 nm
Intensity(a.u)
Wavelength(nm)
Me
N
N
3e

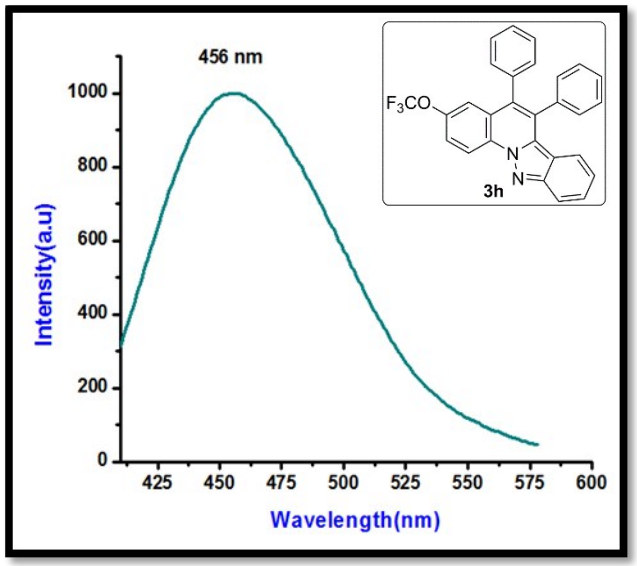

266 nm
381 nm
Absorbance(%)
Wavelength(nm)
MeO
N
N
3f

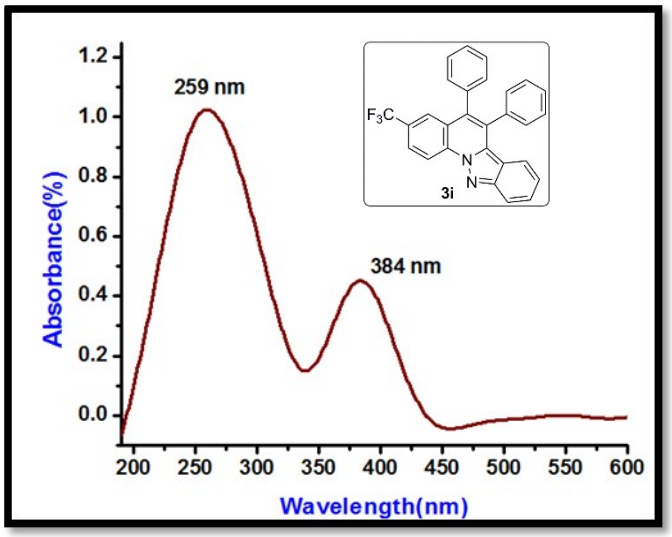

448 nm
Intensity(a.u)
Wavelength(nm)
MeO
N
N
3f

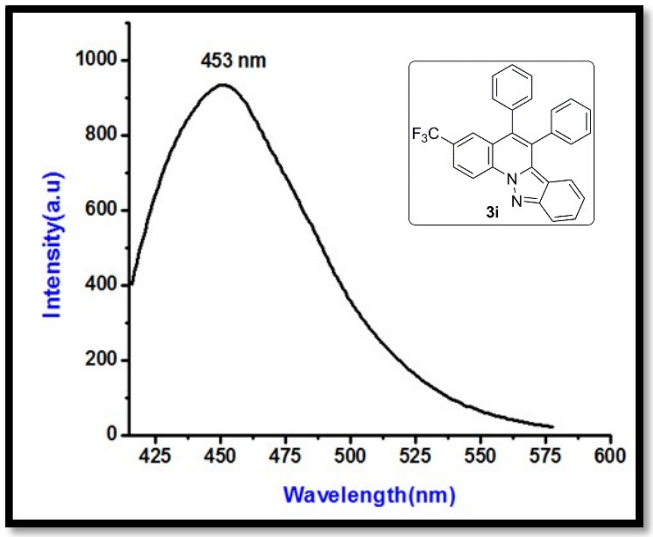

Absorbance(a.u)
Wavelength(nm)
266 nm
375 nm
MeS
3g

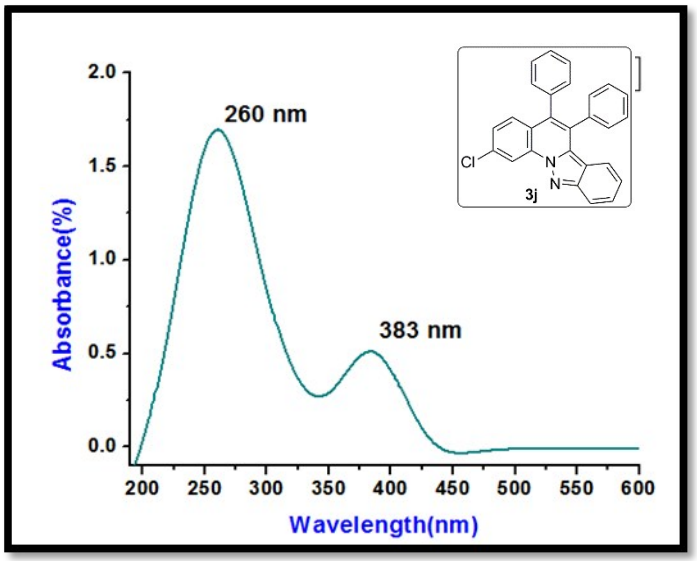

Intensity(a.u)
Wavelength(nm)
448 nm
MeS
3g

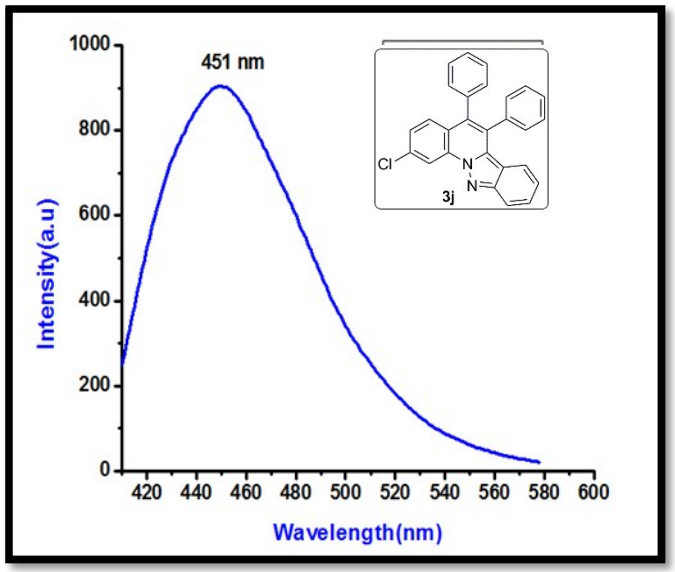

Absorbance(%)
Wavelength(nm)
262 nm
381 nm
F3CO
3h

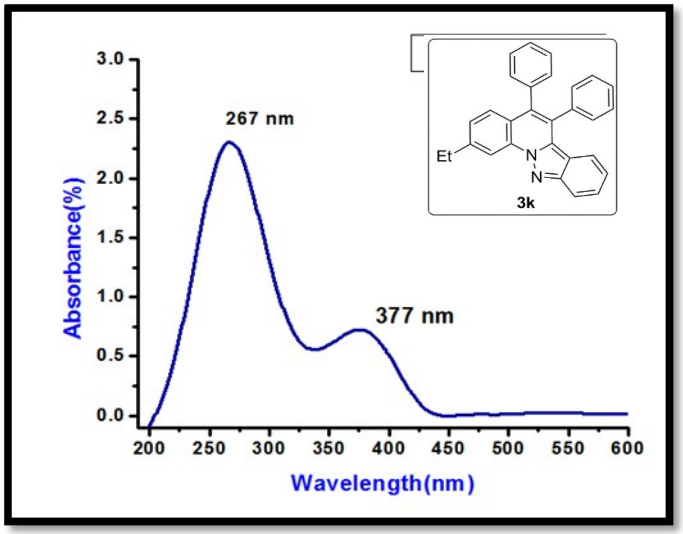

Intensity(a.u)
Wavelength(nm)
456 nm
F3CO
3h

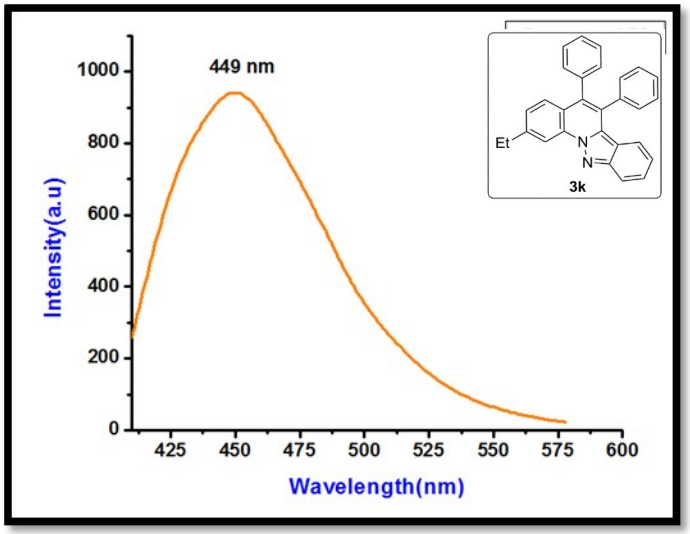

259 nm
384 nm
Absorbance(%)
Wavelength(nm)
3i

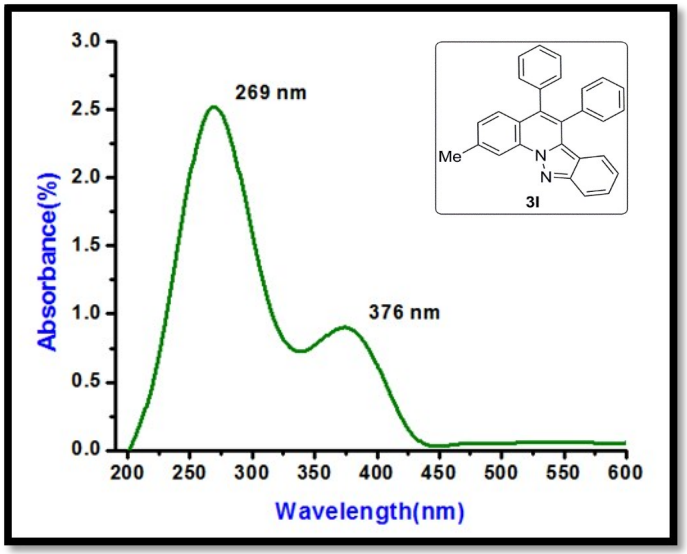

453 nm
Intensity(a.u)
Wavelength(nm)
3i

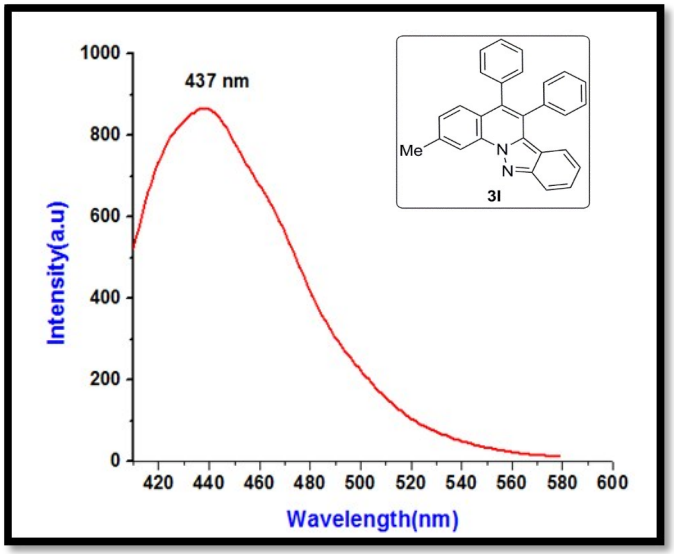

260 nm
383 nm
Absorbance(%)
Wavelength(nm)
3j

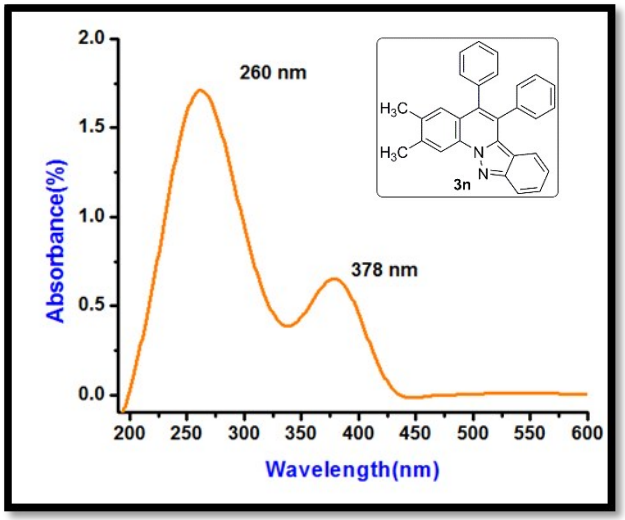

451 nm
Intensity(a.u)
Wavelength(nm)
3j

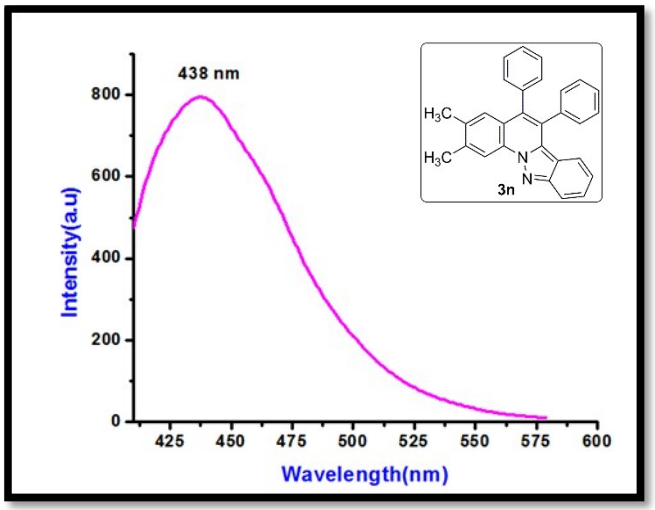

Absorbance(%)
Wavelength(nm)
267 nm
377 nm
Et
N
N
3k

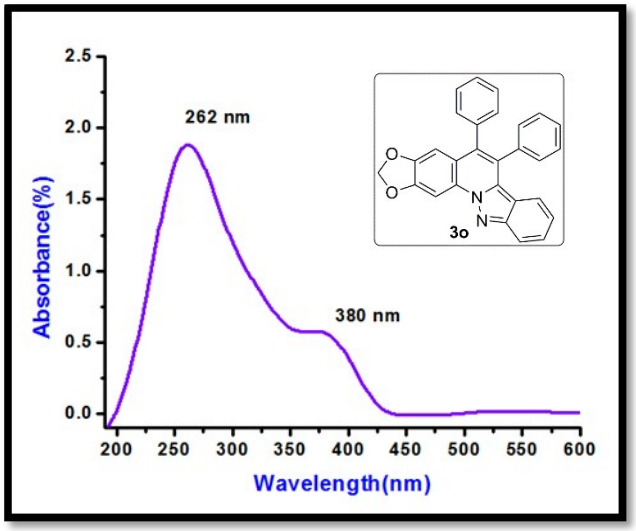

Intensity(a.u)
Wavelength(nm)
449 nm
Et
N
N
3k

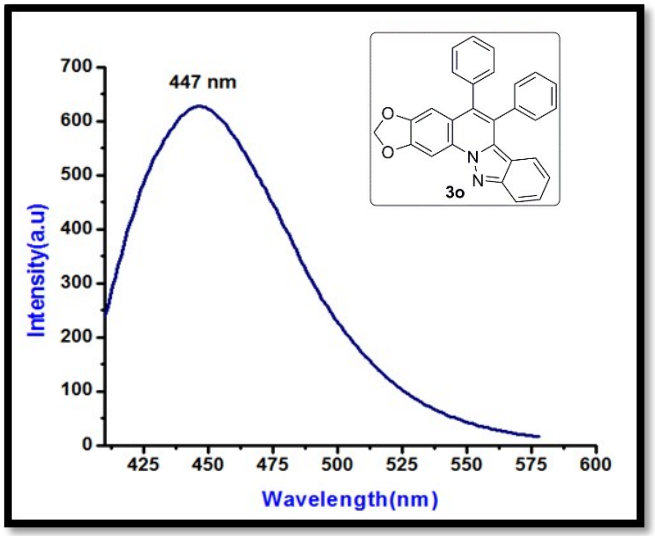

Absorbance(%)
Wavelength(nm)
269 nm
376 nm
Me
N
N
3l

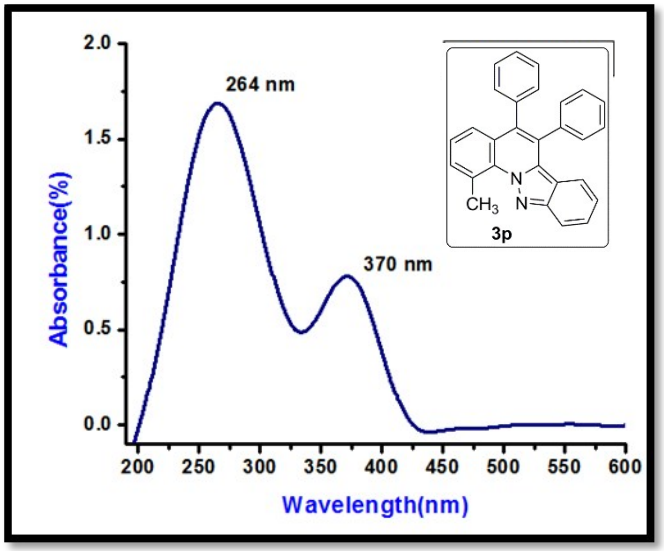

Intensity(a.u)
Wavelength(nm)
437 nm
Me
N
N
3l

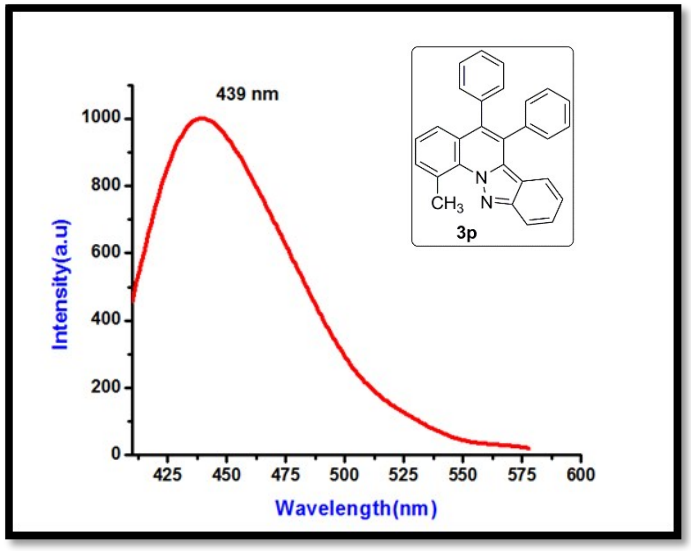

260 nm
378 nm
Absorbance(%)
Wavelength(nm)
3n

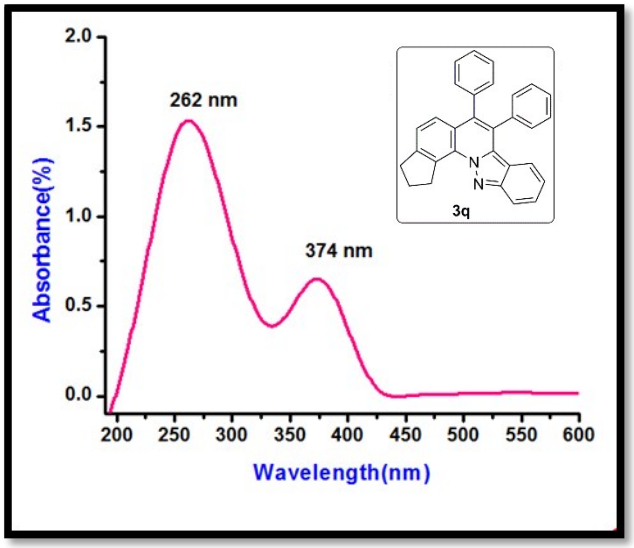

438 nm
Intensity(a.u)
Wavelength(nm)
3n

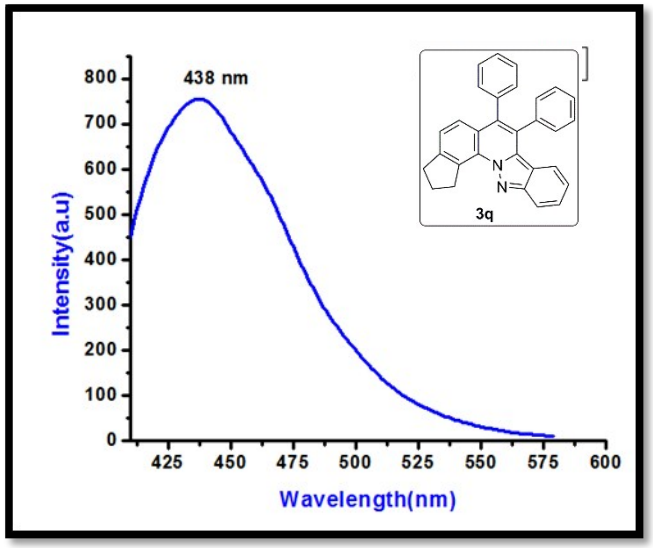

262 nm
380 nm
Absorbance(%)
Wavelength(nm)
3o

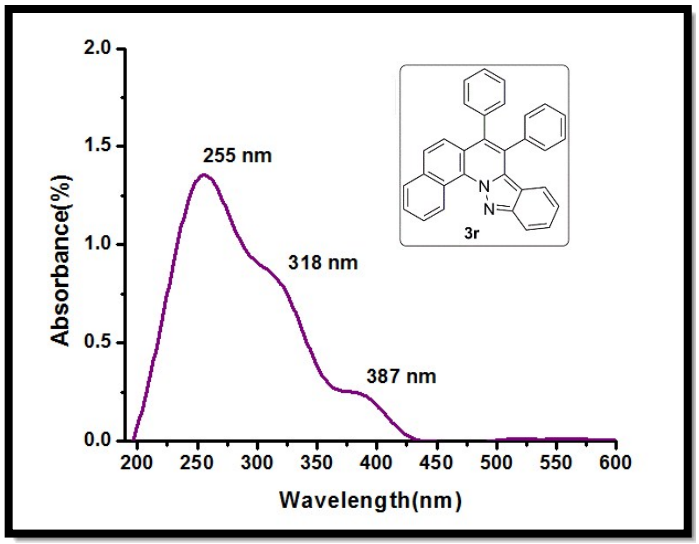

447 nm
Intensity(a.u)
Wavelength(nm)
3o

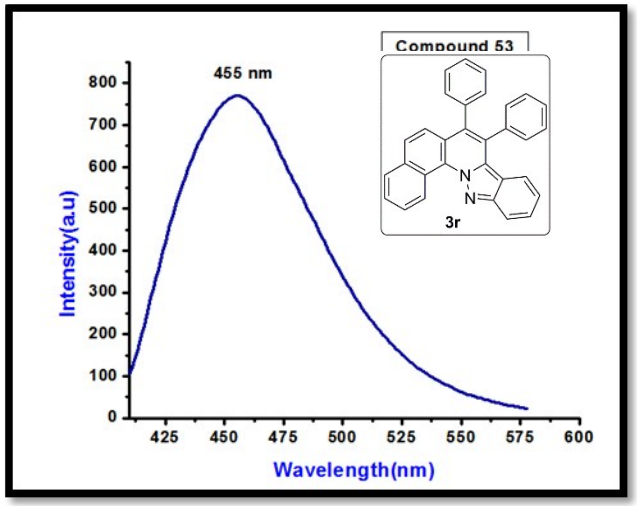

264 nm
370 nm
Absorbance(%)
Wavelength(nm)
3p

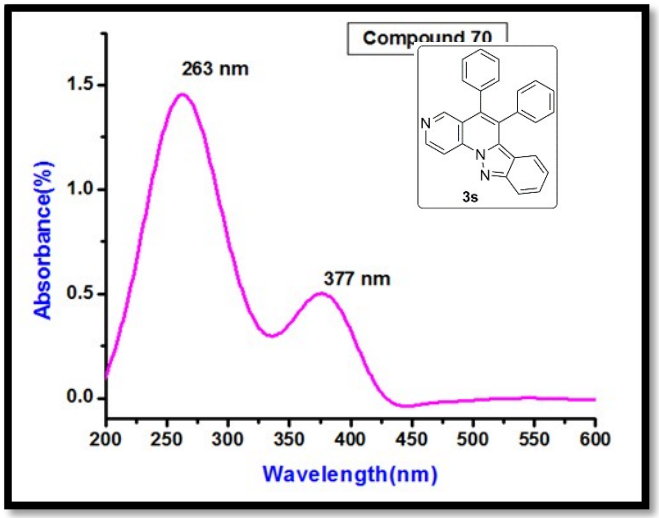

439 nm
Intensity(a.u)
Wavelength(nm)
3p

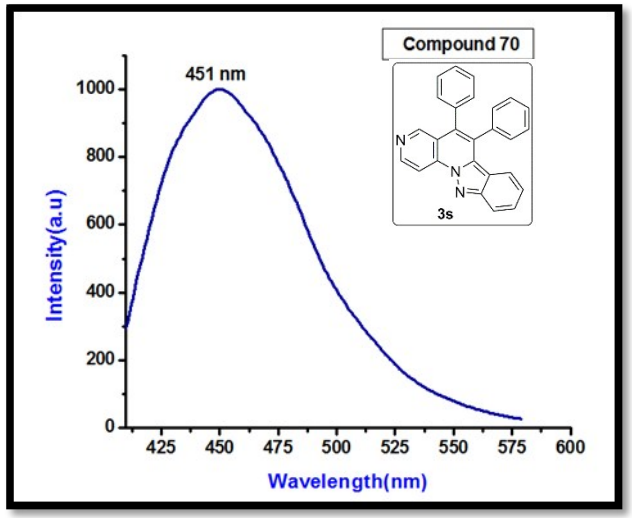

262 nm
374 nm
Absorbance(%)
Wavelength(nm)
3q

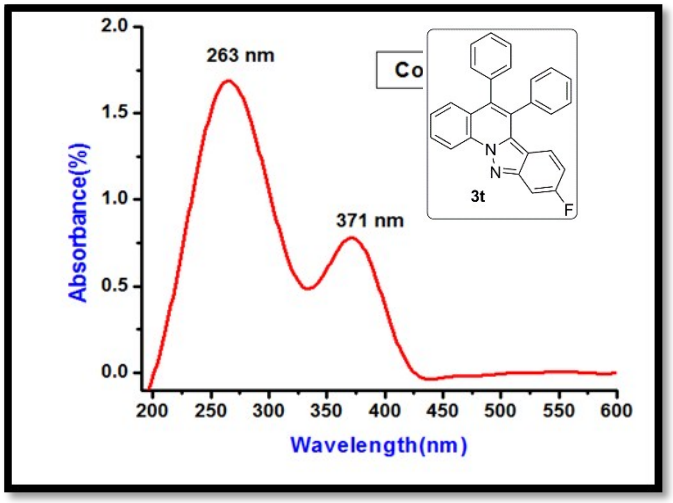

438 nm
Intensity(a.u)
Wavelength(nm)
3q

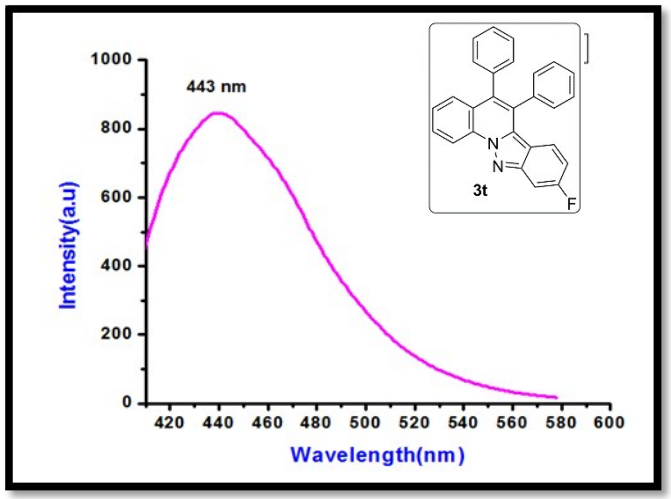

Absorbance(%)
Wavelength(nm)
255 nm
318 nm
387 nm
3r

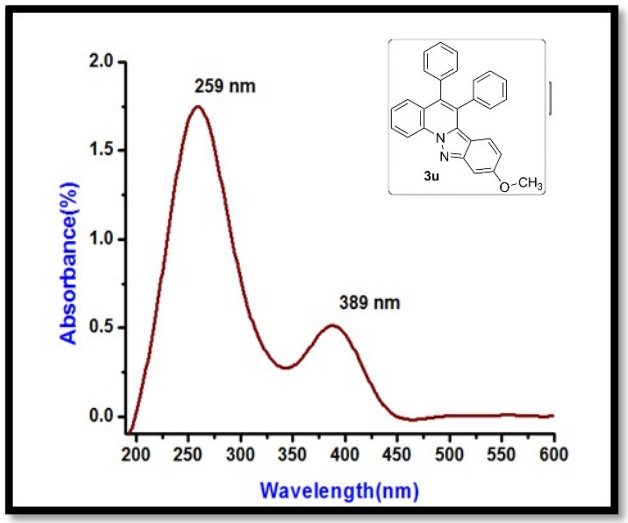

Compound 53
455 nm
Intensity(a.u)
Wavelength(nm)
3r

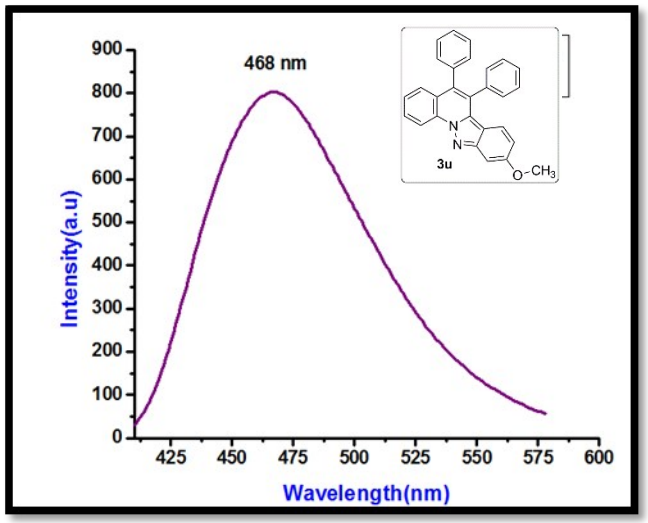

Compound 70
263 nm
377 nm
Absorbance(%)
Wavelength(nm)
3s

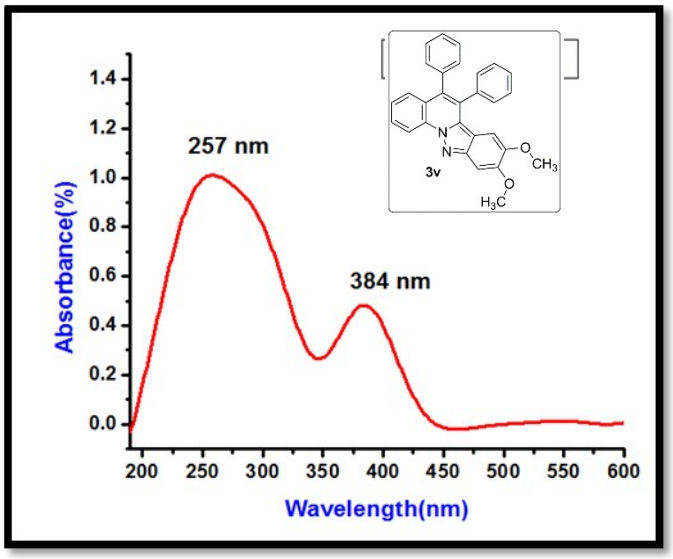

Compound 70
451 nm
Intensity(a.u)
Wavelength(nm)
3s

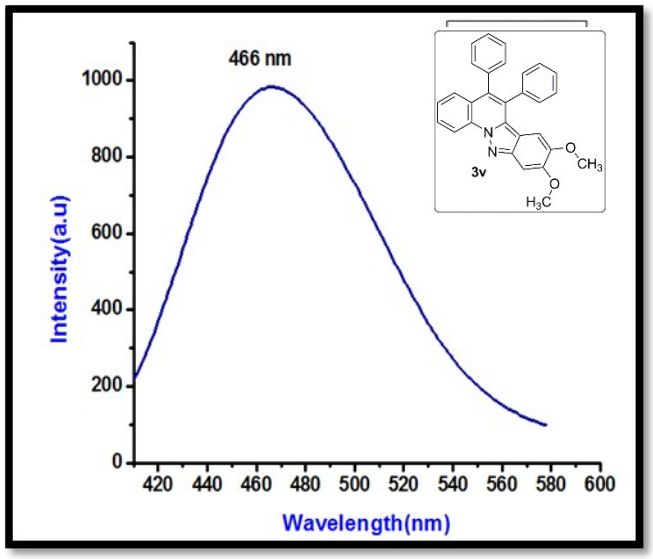

263 nm
371 nm
Co
3t
F
Absorbance(%)
Wavelength(nm)

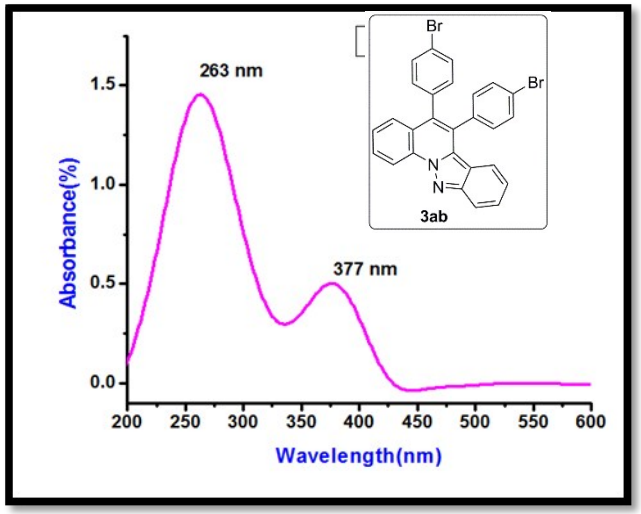

443 nm
3t
F
Intensity(a.u)
Wavelength(nm)

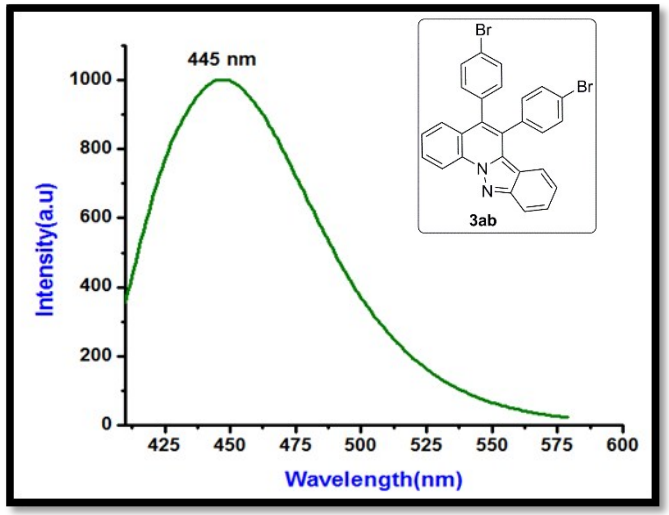

259 nm
389 nm
3u
O-CH3
Absorbance(%)
Wavelength(nm)

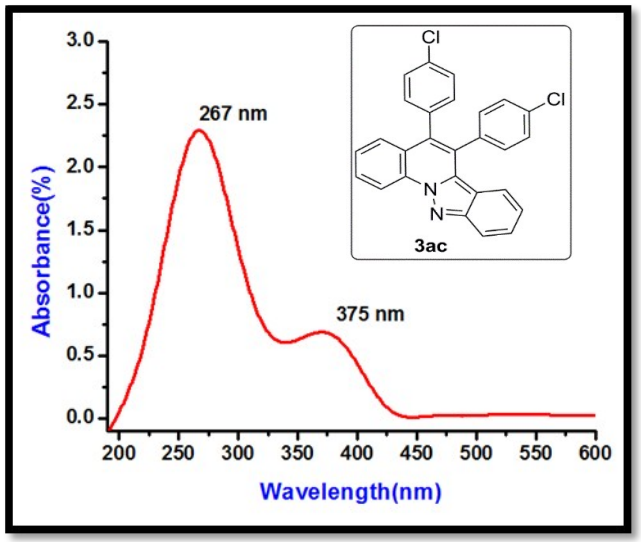

468 nm
3u
O-CH3
Intensity(a.u)
Wavelength(nm)

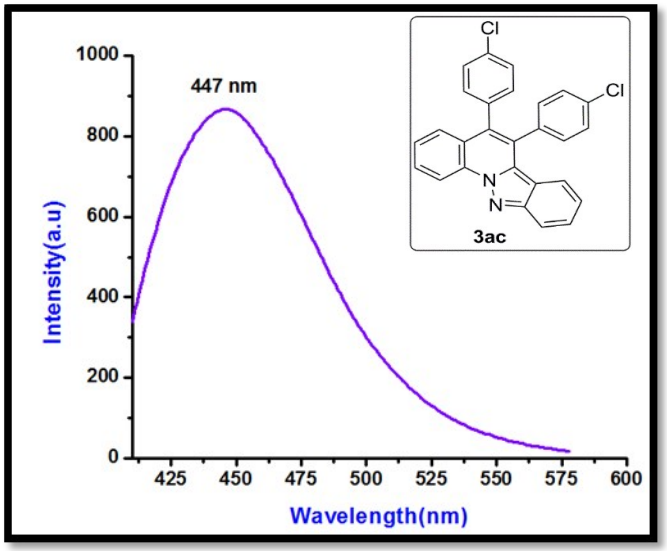

257 nm
384 nm
Absorbance(%)
Wavelength(nm)
3v

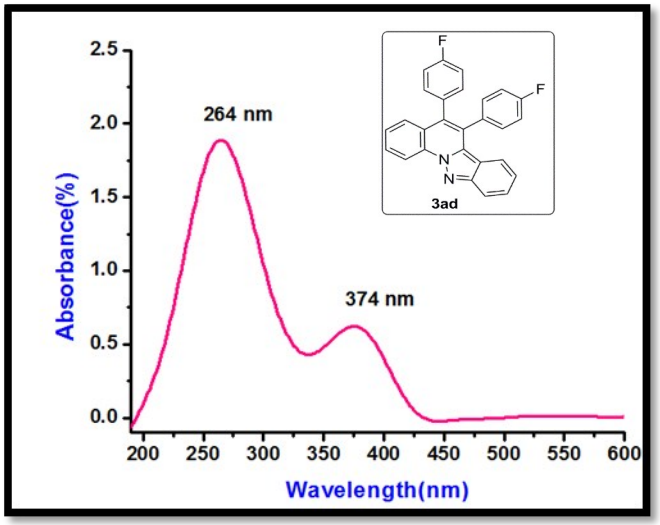

466 nm
Intensity(a.u)
Wavelength(nm)
3v

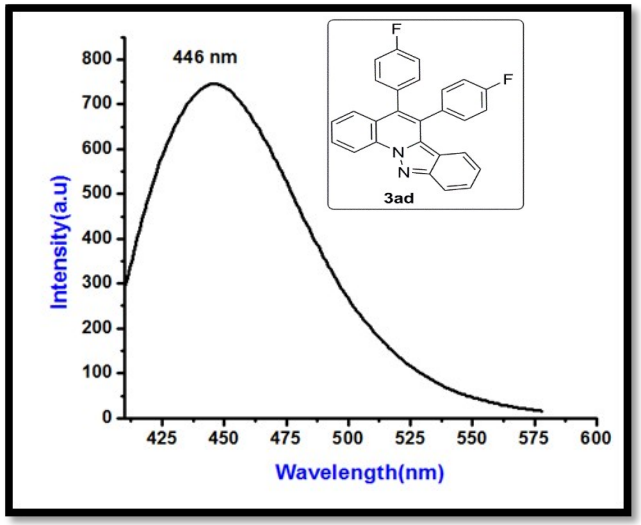

263 nm
377 nm
Absorbance(%)
Wavelength(nm)
3ab

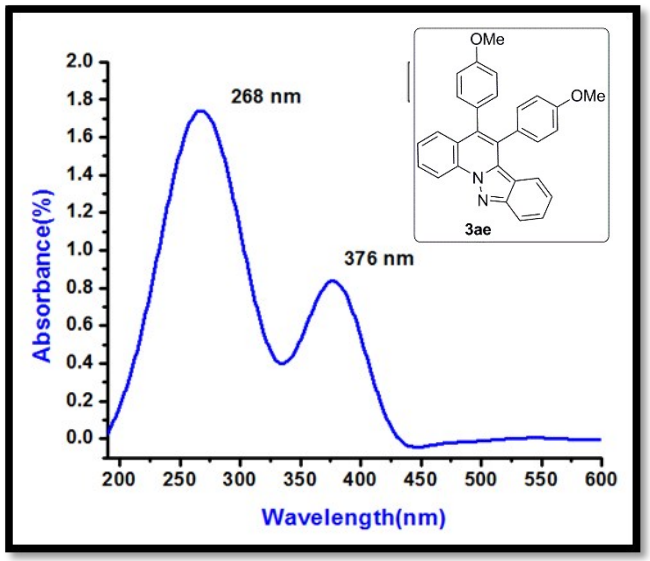

445 nm
Intensity(a.u)
Wavelength(nm)
3ab

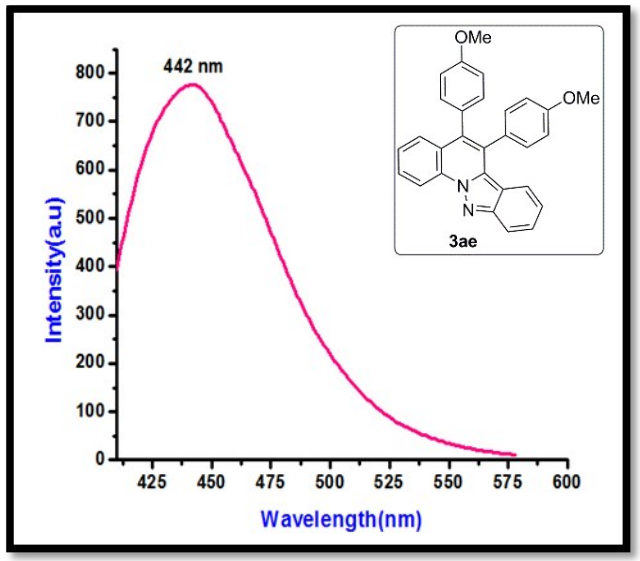

Absorbance(%)
Wavelength(nm)
267 nm
375 nm
Cl
Cl
N
N
3ac

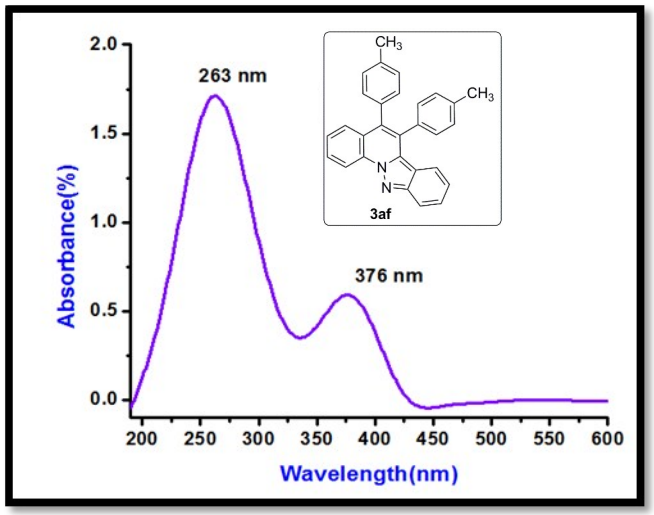

Intensity(a.u)
Wavelength(nm)
447 nm
Cl
Cl
N
N
3ac

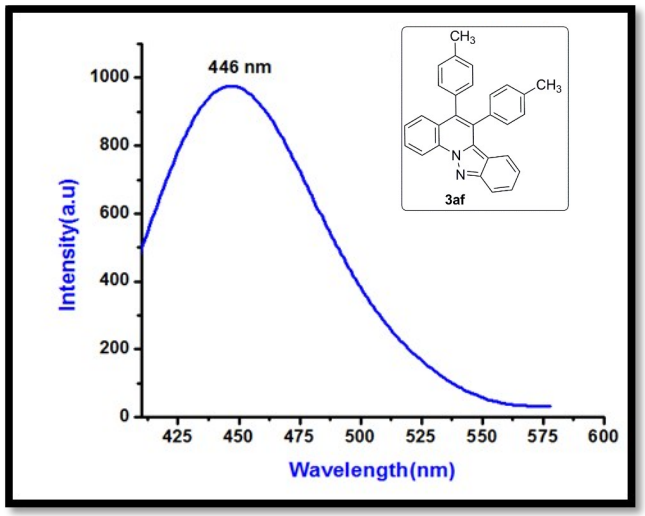

Absorbance(%)
Wavelength(nm)
264 nm
374 nm
F
F
N
N
3ad

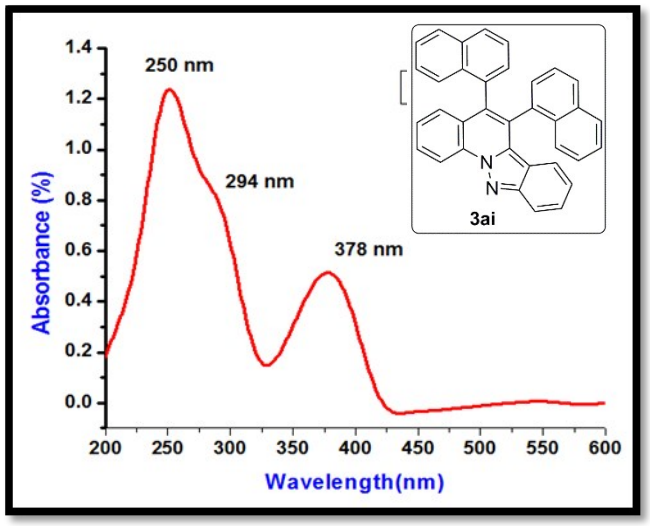

Intensity(a.u)
Wavelength(nm)
446 nm
F
F
N
N
3ad

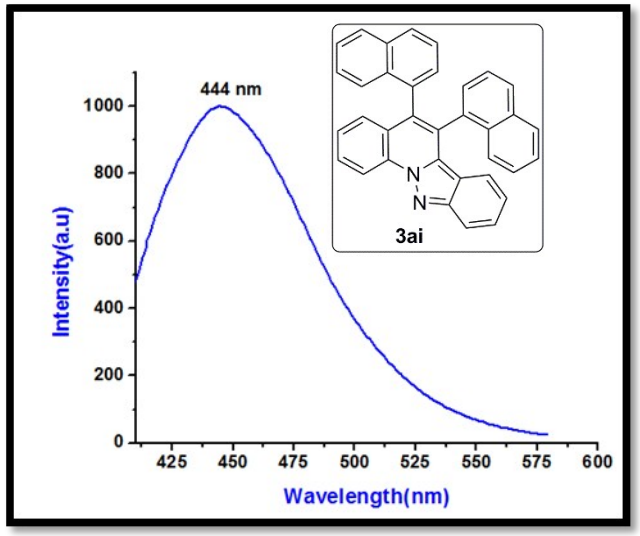

Absorbance(%)
Wavelength(nm)
268 nm
376 nm
OMe
OMe
3ae

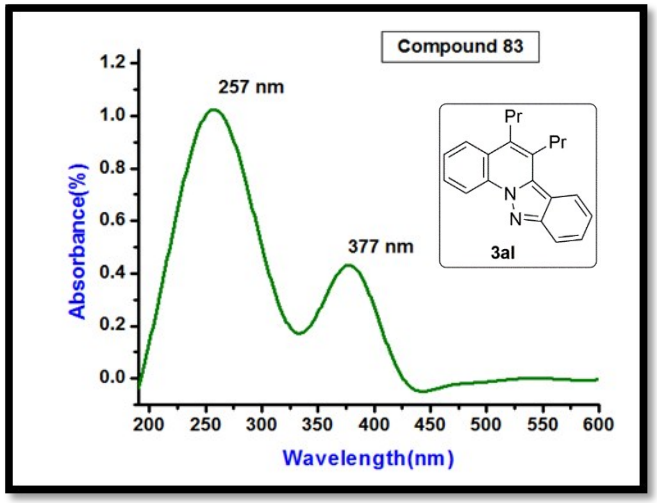

Intensity(a.u)
Wavelength(nm)
442 nm
OMe
OMe
3ae

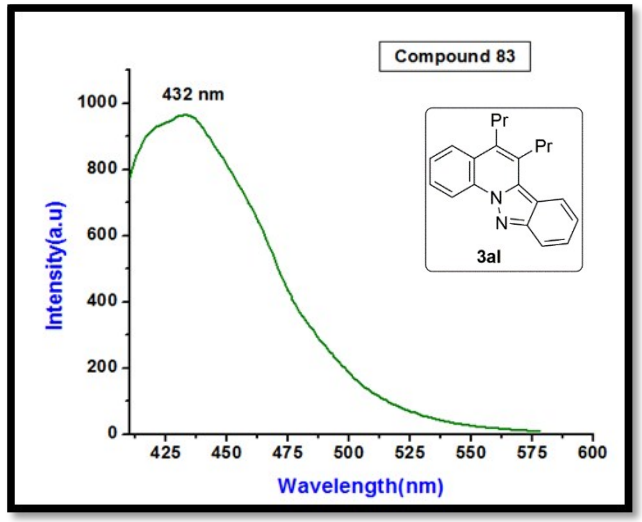

Absorbance(%)
Wavelength(nm)
263 nm
376 nm
CH3
CH3
3af


Intensity(a.u)
Wavelength(nm)
446 nm
CH3
CH3
3af


250 nm
294 nm
378 nm
Absorbance (%)
Wavelength(nm)
3ai


444 nm
Intensity(a.u)
Wavelength(nm)
3ai


Compound 83
257 nm
377 nm
Absorbance(%)
Wavelength(nm)
Pr
Pr
3al


Compound 83
432 nm
Intensity(a.u)
Wavelength(nm)
Pr
Pr
3al